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# Optimal energy supply network determination and life cycle analysis for hybrid coal, biomass, and natural gas to liquid (CBGTL) plants using carbon-based hydrogen production

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ABSTRACT

A mixed-integer linear optimization formulation is developed to analyze the United States energy supply chain network for the hybrid coal, biomass, and natural gas to liquids (CBGTL) facilities. Each state is discretized into octants and each octant centroid serves as a potential location of one facility. The model selects the optimal locations of CBGTL facilities, the feedstock combination, and size of each facility that gives the minimum overall production cost. Two case studies are presented to investigate the effects of various technologies and hydrogen prices. The CBGTL network is capable to supply transportation fuel demands for the country at a cost between \$15.68 and \$22.06/GJ LHV (\$76.55–\$112.91/bbl crude oil) of produced liquid fuels for both case studies. Life cycle analysis on each facility in the supply chain network shows that the United States fuel demands can be fulfilled with an excess of 50% emissions reduction compared to petroleum based processes.

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## 1. Introduction

The United States' high dependence on petroleum, particularly the country's transportation sector, has motivated research efforts to discover alternative sources and processes to fulfill the nation's demand. Additionally, the transportation sector faces challenges to reduce the greenhouse gas (GHG) emissions from the production, distribution, and consumption of liquid fuels. Gasification and Fischer–Tropsch (FT) based processes are among the promising alternatives due to their capabilities in converting more domestically abundant sources, such as coal and biomass, into transportation fuel products. Integrating biomass into fuel producing processes suggests significant potential to remediate the emissions problem, since as a renewable source, biomass can provide the negative carbon emissions from the atmosphere during its growth and cultivation. Herbaceous energy crops, especially, can provide additional $CO_2$ storage from soil sequestration (Larson et al., 2010; Tilman, Hill, & Lehman, 2006). There is, however, an upper limit to how much biomass can be utilized due to the land area constraint in the United States of America. Recently, Baliban, Elia, and Floudas (2010) and Elia, Baliban, and Floudas (2010) proposed a novel hybrid coal, biomass, and natural gas to liquid (CBGTL) process that produces gasoline, diesel, and kerosene in ratios consistent with the United States transportation demands. A hydrogen input is utilized to facilitate a near-100% converstion of feedstock carbon to products via the reverse water-gas-shift (rWGS) reaction. Due to its unique features, namely (i) the $CO_2$ recycle loop to a rWGS reactor, (ii) novel process flowsheet alternatives, and (iii) simultaneous heat and power integration of the complete processes, the CBGTL process' economic performance is competitive with petroleum-based processes.

The costs associated with the CBGTL plant include the high investment costs for its installment, as well as its operational costs, which cover logistical costs for the upstream and downstream phases of the plant activity (i.e., the transportation of feedstocks and products, respectively) and are directly related to its geographical location (Lee & Kwon, 2010; Rentizelas & Tatsiopoulos, 2010). The feasibility of the CBGTL process to fulfill the entire United States demand economically depends on (i) the locations and availabilities of the feedstocks, (ii) the plant sizes, (iii) the plant locations, (iv) the optimal allocation of feedstock to plants, and (v) the optimal allocation of products from plants to product destinations. Trade-offs such as economies of scale due to larger sized, centralized production and the costs of feedstock transportation and product distribution must be considered in an entire energy supply chain framework. To ensure that the transportation sector GHG emissions are reduced, each CBGTL plant will be designed to have a net

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well-to-wheel GHG emissions equal to 50% of a standard petroleum refinery.

The goal of this work is to demonstrate how the CBGTL process can potentially fulfill the whole liquid transportation fuel demand of the country by considering an energy supply chain problem that identifies the optimal energy supply chain network and the most strategic locations for the new CBGTL plants for the United States. A mixed integer linear optimization model is developed to identify the discrete optimal plant locations such that the total network cost is minimized. The solution of the supply chain problem will yield the optimal distribution of the CBGTL plant locations across the country including the plant capacity and specific feedstock types. For every CBGTL plant in the energy supply chain network, the mathematical model will determine the starting location, quantity used, and mode of transportation for each feedstock. Additionally, for every CBGTL plant, the model will determine the final location, quantity shipped, and mode of transportation for each product.

The rest of the paper is organized as follows. Sections 2–5 discuss the data used as inputs to the mathematical model. Section 2 outlines the model input associated with the operation of the CBGTL plants. Section 3 describes the databases that supply information regarding feedstock availabilities for the United States and the assumptions used for this work. Information on fuel demands and the transportation infrastructure for the country are detailed in Sections 4 and 5, respectively. In Section 6, the mathematical model for the CBGTL supply chain network is presented, and the results for the two case studies are discussed in Section 7.

## 2. Novel hybrid coal, biomass, gas to liquid (CBGTL) plants

The CBGTL process follows the description outlined in Baliban et al. (2010) and Elia et al. (2010) Each plant is assumed to process one type of coal, biomass, and natural gas feedstock, producing refined gasoline, diesel, and kerosene. The process is designed such that the ratios of liquid fuel products exiting the plant match those of the United States fuel demands (Baliban et al., 2010). In order to fulfill the entire United States fuel demands, however, a network of CBGTL plants must be constructed that utilizes a variety of coal, biomass, and natural gas resources available in the country. Based on the Quality Guidelines for Energy System Studies published by the DOE/NETL (National Energy Technology Laboratory, 2004) and the EIA's Annual Coal Report 2008 (Energy Information Administration, 2008a), 6 coal types are considered in our analysis, namely lignite, sub-bituminous, high-, medium-, and low-volatile bituminous, and anthracite coal, as possible inputs to the CBGTL process. Biomass feedstocks for energy industry are commonly categorized into agricultural residues and forest residues (Department of Agriculture, 2008; Department of Energy and Department of Agriculture, 2005). Agricultural residues include herbaceous energy crops (e.g., switchgrass), corn stover, and residues from oats, wheat, barley, sorghum bagasse, rice, cotton, soybeans, etc., while forest residues include hardwood and softwood residues, hardmill and softmill wastes, and urban wood wastes (Department of Energy and Department of Agriculture, 2005), giving a total of 15 biomass types considered in the CBGTL energy supply chain network. The compositions of these various biomass types are obtained from the ECN (Energy Research Centre of the Netherlands) Phyllis database (van der Drift & van Doorn, 2002). The natural gas composition is assumed to be generally uniform and the average composition given by the Quality Guidelines for Energy System Studies (National Energy Technology Laboratory, 2004) will be used in our analysis. All the different types of coal and biomass with their respective elemental compositions and heating values can be found in Tables 1 and 2, respectively, and the natural gas composition is presented in Table 3.

Each CBGTL plant is designed to receive one type of each of the biomass, coal, and natural gas feedstocks. Three plant sizes, namely small-, medium-, and large-scale plants with production capabilities, 10,000, 50,000, and 200,000 BPD, respectively, are allowed to be constructed in the energy supply chain network. These capacities are selected apriori based on the current capacities of the refineries in the United States, which range from 2000 to 572,500 BPD (Energy Information Administration, 2009). The distribution of fuel products for each plant size corresponds to 6676.74 BPD, 2160.08 BPD, and 1163.18 BPD of gasoline, diesel, and kerosene products, respectively for small plants, 33,383.72 BPD, 10,800.39 BPD, and 5815.89 BPD of gasoline, diesel, and kerosene products, respectively for medium plants, and 133,534.88 BPD, 43,201.57 BPD, and 23,263.55 BPD of gasoline, diesel, and kerosene products, respectively for large plants.

We introduce an environmental constraint by imposing an overall GHG emission target level for each CBGTL plant. The environmental advantage of co-feeding biomass with the non-renewable resources, namely the negative emissions obtained during the growing and cultivation of the biomass feedstock, is increased with higher relative amount of biomass into the system. An upper limit on the amount of carbon originating from natural gas is set to be 15% of the total carbon input into the system, while the coal and biomass proportions are determined via a life-cycle analysis (Section 2.1) that sets a well-to-wheel emission target for each plant to have 50% reduction of petroleum-based processes, which has been evaluated to emit 91.6 kg $CO_{2eq}$/GJ LHV[1] (lower heating value) fuel produced (Larson et al., 2010). By setting this target, the required amount of coal, biomass, and natural gas feedstock for each plant type can be calculated apriori to produce gasoline, diesel, and kerosene in ratios consistent with United States fuel demands. The complete list of CBGTL plant types with their respective input requirements can be found in the Supporting Information.

Process simulations were completed for each combination of coal, biomass, and natural gas type, and the considered plant capacities, giving a total of 270 different simulations (i.e., 15 biomass types × 6 coal types × 1 natural gas type × 3 plant sizes = 270 simulations) using the Aspen Plus software based on the approach of Baliban et al. (2010) and Elia et al. (2010). The overall mass balance information of each CBGTL plant, which includes (i) the amount of feedstock that needs to be delivered to the plant, (ii) the amount of products that each plant produces, (iii) the hydrogen requirement for the reverse water gas shift reaction, and (iv) the electricity requirements for the plant operation, is extracted from the simulation results.

Additionally, the Aspen Plus simulations provide information on the sizes of each plant unit. The investment costs of constructing a new CBGTL plant are calculated using capital cost estimates based on literature sources (see Table 4) and our prior work (Baliban et al., 2010; Elia et al., 2010). Each unit is scaled based on the stream flows from the Aspen Plus simulations, and the balance of plant and indirect cost factors are incorporated in the total overnight cost (TOC) using the following equation:

$$TOC = (1 + IC) \cdot (1 + BOP) \cdot C_o \cdot \left(\frac{S}{S_o}\right)^{sf} \cdot n^{0.9} \qquad (1)$$

where $C_o$ is the base cost, $S_o$ is the base capacity, $S$ is the actual capacity, $n$ is the total number of trains, $sf$ is the cost scaling factor,

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[1] The total amount of greenhouse gases produced is expressed in terms of $CO_2$ mass equivalent. This reduction is in accordance with the target to achieve 50% reduction in global emissions by 2050, as agreed by the international leaders at the G8 summit (G8, 2008). The emissions of various greenhouse gases are converted using their respective global warming potentials (Argonne National Laboratory, 2007).

**Table 1**
Properties of the six coal types considered in the energy supply chain network. Compositions of lignite, sub-bituminous, high-, med-, and low-volatile bituminous coals are obtained from the Annual Coal Report 2008 (Energy Information Administration, 2008a) and the composition for anthracite coal is obtained from the ECN Phyllis database (van der Drift & van Doorn, 2002).

| Coal type | Proximate analysis (db, wt%) | | | | Ultimate analysis (db, wt%) | | | | | | Heating values | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Moist. (ar) | Ash | VM [a] | FC [b] | C | H | N | Cl | S | O | HHV [c] (kJ/kg) | LHV [d] (kJ/kg) |
| Lignite | 32.24 | 9.72 | 44.94 | 44.54 | 65.85 | 4.36 | 1.04 | 0.04 | 0.8 | 18.19 | 25,588 | 24,625 |
| Sub-bituminous | 28.09 | 8.77 | 44.73 | 45.87 | 68.43 | 4.88 | 1.02 | 0.03 | 0.63 | 16.24 | 27,254 | 26,176 |
| High-volatile bituminous | 7.97 | 15.48 | 40.05 | 39.64 | 65.65 | 4.23 | 1.16 | 0.05 | 4.83 | 8.6 | 27,798 | 26,864 |
| Med-volatile bituminous | 1.13 | 13.18 | 27.45 | 57.05 | 74.23 | 4.08 | 1.35 | 0 | 2.32 | 4.84 | 31,324 | 30,423 |
| Low-volatile bituminous | 0.65 | 4.77 | 18.6 | 75.97 | 86.71 | 4.23 | 1.27 | 0.19 | 0.66 | 2.17 | 34,946 | 34,012 |
| Anthracite | 1.9 | 2.9 | 7.7 | 89.4 | 88.9 | 3.4 | 1.55 | 0.082 | 0.81 | 2.3 | 34,600 | 33,858 |

ar: as received; db: dry basis.

[a] Volatile matters.

[b] Fixed carbon.

[c] Higher heating value.

[d] Lower heating value.

**Table 2**
Properties of the sixteen biomass types considered in the energy supply chain model, categorized into perennial grasses, agricultural residues, and forest residues. Compositions of all biomass types are obtained from the ECN Phyllis database (van der Drift & van Doorn, 2002).

| Biomass type | Proximate analysis (db, wt%) | | | | Ultimate analysis (db, wt%) | | | | | | Heating values | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Moist. (ar) | Ash | VM [a] | FC [b] | C | H | N | Cl | S | O | HHV [c] (kJ/kg) | LHV [d] (kJ/kg) |
| *Perennial grasses* | | | | | | | | | | | | |
| Switchgrass | 8.2 | 4.6 | 79.2 | 16.2 | 46.9 | 5.85 | 0.58 | 0.501 | 0.11 | 41.5 | 18,636 | 17,360 |
| *Agricultural residues* | | | | | | | | | | | | |
| Corn stover | 6.1 | 5.1 | 80.9 | 14 | 46.8 | 5.74 | 0.66 | 0.266 | 0.11 | 41.4 | 18,101 | 16,849 |
| Oat straw | 8.2 | 5.9 | 80.5 | 13.6 | 47.6 | 5.8 | 0.5 | 0.09 | 0.08 | 43.5 | 18,940 | 17,674 |
| Wheat straw | 9.7 | 5.8 | 78.7 | 15.5 | 46.7 | 5.73 | 0.71 | 0.255 | 0.11 | 40.6 | 18,580 | 17,330 |
| Barley straw | 6.2 | 4.3 | 76.8 | 18.9 | 45.9 | 5.92 | 0.43 | 0.352 | 0.2 | 43 | 18,145 | 16,854 |
| Sorghum bagasse | 10.7 | 8.1 | 73.4 | 18.5 | 39.5 | 7.51 | 1.1 | 0.604 | 0.22 | 43 | 17,894 | 16,255 |
| Rice straw | 7.9 | 18.7 | 65.5 | 15.8 | 38.2 | 5.2 | 0.87 | 0.58 | 0.18 | 36.3 | 15,086 | 13,951 |
| Cotton | 10.3 | 9.4 | 82.2 | 8.4 | 49 | 4.71 | 1.45 | 0 | 0.36 | 35.1 | 16,270 | 15,241 |
| Soybeans | 6.3 | 5.1 | 19 | 75.9 | 43.1 | 6.36 | 0.85 | 0 | 0.09 | 44.5 | 18,170 | N/A |
| Generic residue | 10 | 5.9 | 72.36 | | 47.08 | 5.87 | 1.16 | 0.08 | 1.16 | 39.77 | 14,379 | 13,068 |
| *Forest residues* | | | | | | | | | | | | |
| Urban wood waste | 14.9 | 3.2 | N/A | N/A | 51.6 | 6.33 | 1.45 | 0 | 0.22 | 36.6 | 20,143 | 18,762 |
| Hardwood residue | 45 | 2.14 | N/A | N/A | 50.19 | 5.9 | 0.32 | 0 | 0.03 | 41.42 | 19,130 | 17,842 |
| Softwood residue | 45 | 0.3 | 80.1 | 19.6 | 50.91 | 6.06 | 0.03 | 0 | 0.01 | 42.69 | 19,590 | 18,267 |
| Hardmill waste | 20 | 2.14 | N/A | N/A | 50.19 | 5.9 | 0.32 | 0 | 0.03 | 41.42 | 19,130 | 17,842 |
| Softmill waste | 20 | 0.3 | 80.1 | 19.6 | 50.91 | 6.06 | 0.03 | 0 | 0.01 | 42.69 | 19,590 | 18,267 |

ar: as received; db: dry basis.

[a] Volatile matters.

[b] Fixed carbon.

[c] Higher heating value.

[d] Lower heating value.

*BOP* is the balance of plant (BOP) percentage, and *IC* is the indirect cost (IC) percentage. *BOP* is calculated as a function of the higher heating value of the biomass feedstock (Larson, Jin, & Celik, 2009) using Eq. (2), and thus will take a different value for every CBGTL plant type (i.e., every feed combination and plant size):

$$BOP(\%) = \frac{0.8867}{MW_{HHV}{}^{0.2096}} \tag{2}$$

**Table 3**
Natural gas composition (National Energy Technology Laboratory, 2004).

| Component | Volume % |
|---|---|
| Methane, $CH_4$ | 93.1 |
| Ethane, $C_2H_6$ | 3.2 |
| Propane, $C_3H_8$ | 0.7 |
| n-Butane, $C_4H_{10}$ | 0.4 |
| Carbon dioxide, $CO_2$ | 1.0 |
| Nitrogen, $N_2$ | 1.6 |
| HHV [a] (MJ/scm) | 38.46 |
| LHV [b] (MJ/scm) | 34.71 |

[a] Higher heating value.

[b] Lower heating value.

Finally, the levelized cost of the CBGTL plant is obtained using the following equation:

$$\text{Levelized cost} = \frac{TOC \cdot (\text{capital charge rate} + \text{operation and maintenance rate})}{365} \tag{3}$$

where the capital charge rate is taken to be 15.41%/year of TOC and the operation and maintenance rate is 4.00%/year of TOC. Electricity is assumed to be available at \$0.07/kWh and is based on the average cost delivered to the industrial sector in 2008 (Energy Information Administration, 2010d). All cost figures are expressed in terms of 2009 Q4 US dollars using the GDP implicit price deflator (US Government Printing Office, 2009).

### 2.1. Life cycle analysis

To evaluate the process' environmental performance, we conduct a well-to-wheel life-cycle analysis for each plant type based on assumptions in the Greenhouse gases, Regulated Emissions, and

**Table 4**
Base capacities, costs (2009 $), and scaling factors for various process units in the CBGTL process.

| Unit name | $C_o$ (MM$) | Flow units | $S_o$ | $S_{\max}$ | *sf* | Indirect costs | Ref. |
|---|---|---|---|---|---|---|---|
| Biomass H&D [a] | 3.702 | wet tonne/day | 1550.40 | – | 0.77 | 32.0% | Larson et al. (2009) |
| Biomass Gasifier | 7.486 | dry tonne/day | 1000.80 | 2880 | 0.7 | 32.0% | Larson et al. (2009) |
| Ash Cyclone | 1.063 | actual m$^3$/s | 68.7 | 180 | 0.7 | 32.0% | Larson et al. (2009) |
| Tar Cracker | 0.855 | actual m$^3$/s | 47.1 | 52 | 0.7 | 32.0% | Larson et al. (2009) |
| Ceramic Filter | 21.724 | actual m$^3$/s | 14.4 | – | 0.65 | 32.0% | Larson et al. (2009) |
| Coal Storage & Handling [b] | 34.72 | tonne/day | 2367 | – | 0.67 | Included | Kreutz, Williams, Consonni, and Chiesa (2005) |
| Coal Gasifier [b] | 172.17 | tonne/day | 2479.7 | – | 0.67 | Included | Kreutz et al. (2005) |
| RGS | 0.923 | standard m$^3$/s | 0.315 | 3.146 | 0.7 | 32.0% | Larson et al. (2009) |
| COS/HCN Hydrolyzer | 3.058 | tonne/day | 4922.78 | 7228.5 | 0.67 | 32.0% | National Energy Technology Laboratory (2007) |
| Acid Gas Removal Unit | 23.359 | standard m$^3$/s | 55.556 | – | 0.65 | 32.0% | Larson et al. (2009) |
| Fischer–Tropsch | 12.26 | standard m$^3$/s | 19.822 | – | 0.72 | 32.0% | Larson et al. (2009) |
| Hydrocarbon Recovery | 0.65 | tonne/day | 157.20 | 2177.28 | 0.7 | 32.0% | Larson et al. (2009) |
| Wax Hydrocracker | 8.42 | tonne/day | 97.803 | 6259.68 | 0.7 | 32.0% | Larson et al. (2009) |
| Distillate Hydrotreater | 2.25 | tonne/day | 31.255 | 7076.16 | 0.7 | 32.0% | Larson et al. (2009) |
| Naphtha Hydrotreater | 0.68 | tonne/day | 22.317 | 7076.16 | 0.7 | 32.0% | Larson et al. (2009) |
| Kerosene Hydrotreater | 2.25 | tonne/day | 31.255 | 7076.16 | 0.7 | 32.0% | Larson et al. (2009) |
| Naphtha Reformer | 4.70 | tonne/day | 37.340 | 8164.80 | 0.7 | 32.0% | Larson et al. (2009) |
| C5/C6 Isomerizer | 0.86 | tonne/day | 12.606 | 2721.00 | 0.7 | 32.0% | Larson et al. (2009) |
| C3/C4/C5 Alkylation Unit | 52.293 | tonne/day | 1092.32 | – | 0.7 | 32.0% | Bechtel (1992, 1998) |
| C4 Isomerizer | 9.497 | tonne/day | 537.211 | – | 0.7 | 32.0% | Bechtel (1992, 1998) |
| Saturated Gas Plant | 7.830 | tonne/day | 365.816 | – | 0.7 | 32.0% | Bechtel (1992, 1998) |
| Auto-Thermal Reactor | 31.02 | standard m$^3$/s | 119.611 | 2621.600 | 0.67 | 32.0% | Kreutz et al. (2008) |
| Air Separation Unit [b] | 41.58 | tonne/day $O_2$ | 1838.40 | – | 0.5 | 27.0% | Larson et al. (2009) |
| Claus Plant [b] | 27.32 | tonne/day S | 81 | – | 0.67 | Included | Kreutz et al. (2005) |
| *Compressors* [b] | | | | | | | |
| $CO_2$ Compressor | 5.55 | MW | 10 | – | 0.67 | 32.0% | Larson et al. (2009) |
| Acid Gas Compressor | 5.64 | MW | 10 | – | 0.67 | 32.0% | Larson et al. (2009) |
| FT Feed Compressor | 5.64 | MW | 10 | – | 0.67 | 32.0% | Larson et al. (2009) |
| ATR Compressor | 5.64 | MW | 10 | – | 0.67 | 32.0% | Larson et al. (2009) |
| Plant Fuel Compressor | 5.64 | MW | 10 | – | 0.67 | 32.0% | Larson et al. (2009) |
| Sour Gas Compressor | 5.64 | MW | 10 | – | 0.67 | 32.0% | Larson et al. (2009) |
| Air Compressor | 4.84 | MW | 10 | – | 0.67 | 32.0% | Larson et al. (2009) |
| $O_2$ Compressor | 6.47 | MW | 10 | – | 0.67 | 32.0% | Larson et al. (2009) |
| Claus Recycle Compressor | 5.64 | MW | 10 | – | 0.67 | 32.0% | Larson et al. (2009) |
| Steam Turbines [b] | 53.14 | MW | 136 | – | 0.67 | 27.0% | Larson et al. (2009) |
| Heat Exchanger Network (estimated) | 48.12 | MW | 355 | – | 1 | 27.0% | Larson et al. (2009) |
| SMR [b] | 284.977 | kg/s $H_2$ | 12.7435 | – | 0.75 | Included | National Research Council (2004) |

[a] Handling and Drying.
[b] BOP included in the cost figures.

Energy use in Transportation (GREET) model (Argonne National Laboratory, 2007). GHG emissions from processes upstream (e.g., cultivation of biomass, mining and gathering of coal and natural gas) and downstream (e.g., transportation and consumption of liquid fuel products) of the CBGTL facilities are included in the calculation to give an overall figure of GHG emissions associated with the CBGTL process. The specific segments that affect the overall emissions are: (a) biomass, coal, and natural gas acquisitions, (b) transportation of feedstock from their source locations to the plant facility, (c) carbon storage in the biomass feedstock, (d) carbon storage in the soil and root during biomass cultivation, (e) hydrogen and electricity production, (f) the CBGTL process, (g) transportation and distribution of products, and (h) consumption of fuel products. A complete sample calculation for the life cycle analysis in this study is presented in Appendix A.

Biomass utilization in the production of transportation fuels provides negative emissions in the overall fuel life cycle due to the carbon accumulation via photosynthesis during its cultivation period. Herbaceous crops are assumed to grow on degraded, carbon-deficient soil, so an additional carbon soil storage benefit of 31.3% kg carbon/kg dry biomass can be claimed (Tilman et al., 2006). The CBGTL process vents 0.5% of its total carbon input and the fuel products are assumed to be fully combusted upon consumption with all of its carbon contents ending up in the atmosphere, which is also the highest contributing factor to GHG emissions in the entire fuel life cycle.

We note that the life cycle analysis for each CBGTL facility was completed in two distinct phases in the study. In the first phase, a life cycle analysis calculation was completed to determine the amount of biomass needed to achieve an overall emissions of 45.8 kg $CO_{2eq}$/GJ LHV fuel produced (i.e., 50% reduction of petroleum-based processes). To complete the life cycle calculation of the fuels and obtain the required amount of biomass, assumptions on the distances traveled and the emissions associated with the transportation of feedstock and products were introduced. Average distance values per each mode of transportation from the GREET model were used to calculate the transportations emissions and the detailed description can be found in Appendix A. Additionally, hydrogen is assumed to be produced from natural gas, electricity is assumed to be produced from coal, and the fuel products are assumed to be transported via interstate pipelines and distributed via intrastate pipelines to the final demand locations.

In the second phase and more specifically in the optimization model, this average distance assumption was removed. Instead, the distance traveled for feedstock and product transportation is calculated based on the origin and destination locations selected by the model. Emissions due to hydrogen production depend on the selected feedstocks and technology. A final life cycle analysis for each plant is conducted to obtain the emissions figures based the optimization model solution and the calculation steps are outlined in Appendix A. All emission values are normalized on a per GJ LHV fuel produced basis.

In addition to environmental emissions, the depletion of feedstock resources must be accounted to ensure the sustainability of the energy supply chain network. Agricultural biomass feedstock is part of the leftover residue remaining after crop harvest, while the perennial grass or dedicated energy crop is assumed to be completely harvested for use as an energy feedstock (Department of Energy and Department of Agriculture, 2005). Removal of these biomass feedstocks is considered to be annually sustainable with no resource depletion (Department of Energy and Department of Agriculture, 2005). The availability of these feedstocks is based on the “high-yield with land use change” scenario (Department of Energy and Department of Agriculture, 2005), which considers that both the removal of crop residues and the introduction of dedicated energy crops will not have an effect on the availability of food from agricultural crops. The forest biomass feedstocks consist either of timber residues, mill wastes, or municipal solid waste, and are also harvested sustainably (Department of Energy and Department of Agriculture, 2005).

The fossil fuel inputs (i.e., coal and natural gas) to the CBGTL process will have a finite timeline for use as feedstocks. Specifically, coal is assumed to be mined using a 100 year lifecycle and natural gas is extracted using a 50 year lifecycle. In future years, it is possible that other energy sectors (e.g., electric power) may need to utilize increasing amounts of fossil fuels, which can place additional demands on both the availability and price of these feedstocks for the CBGTL process. If necessary, the hybrid CBGTL plants can be easily altered to account for a larger input of biomass feedstock while maintaining a competitive price of liquid fuels (Baliban et al., 2010; Elia et al., 2010).

### 2.2. Facility locations

To determine the candidate locations for CBGTL plants, each state is discretized into octants using the following scheme. Initially, each state centroid is obtained by calculating the geometric center of all counties that are associated with the given state. Based on the state centroid, the heading for each county in the state is calculated and the counties are then grouped based on their heading. The candidate locations for the CBGTL plants are located at the centroids of state discretizations.

Two factors are defined, $D1$ and $D2$ in the following equations:

$$D1 = \cos(Lat_s)\cdot\sin(Lat_c) - \sin(Lat_s)\cdot\cos(Lat_c)\cdot\cos(Long_c - Long_s) \tag{4}$$

$$D2 = \sin(Long_c - Long_s)\cdot\cos(Lat_s) \tag{5}$$

where $Lat_s$ and $Long_s$ are the latitude and longitude of state centroid $s$, respectively, and $Lat_c$ and $Long_c$ are the latitude and longitude of county $c$, respectively. Based on these two factors, the heading of each county is determined as follows:

$$D2 \geq 0 \quad D1 \geq 0 \quad \text{Heading} = \arctan\left(\frac{D2}{D1}\right) \tag{6}$$

$$D1 \leq 0 \quad \text{Heading} = 180 + \arctan\left(\frac{D2}{D1}\right) \tag{7}$$

$$D1 = 0 \quad \text{Heading} = 90 \tag{8}$$

$$D2 \leq 0 \quad D1 \geq 0 \quad \text{Heading} = 360 + \arctan\left(\frac{D2}{D1}\right) \tag{9}$$

$$D1 \leq 0 \quad \text{Heading} = 180 + \arctan\left(\frac{D2}{D1}\right) \tag{10}$$

$$D1 = 0 \quad \text{Heading} = 270 \tag{11}$$

$$D2 = 0 \quad D1 \geq 0 \quad \text{Heading} = 0 \tag{12}$$

$$D1 \leq 0 \quad \text{Heading} = 180 \tag{13}$$

$$D1 = 0 \quad \text{Heading} = 0 \tag{14}$$

The counties are grouped into eight octants based on their headings. The octant centroids are then calculated by averaging the longitude and latitude of all counties that belong to a particular octant. The set of valid octants is defined as all octants that have at least one county centroid in its region. It should be noted that some states have less than eight discretizations due to the few number of counties in their regions. The layout of the possible CBGTL plant locations is displayed in Fig. 1.

## 3. Feedstock availability

The placement of the CBGTL plant facilities is strongly dependent on the availability, location, and transportation of the necessary raw materials, amount of demand, and the transportation of desirable products throughout the country. The major inputs to the CGBTL process are coal, biomass, natural gas, hydrogen, and electricity. In this paper, we specifically focus on coal, biomass, and natural gas and their impact on the overall energy supply chain network. It is anticipated that hydrogen production facilities (e.g., biomass, coal, natural gas, solar, and wind) will be constructed in tandem with the CBGTL facilities to provide the necessary input for the reverse water-gas-shift reaction (see case study 2). A series of published nationwide databases on the supply and the process of the three feedstocks are compiled and analyzed in this study, as described by the following subsections.

### 3.1. Coal

The Energy Information Administration (EIA) 2008 Annual Coal Report (Energy Information Administration, 2008a) contains information on the production, cost, and estimate recoverable reserves of four different types of coal (i.e., bituminous, subbituminous, lignite, and anthracite) throughout the country. Using Tables 2 and 6 of Energy Information Administration (2008a), the total production for each coal type can be determined on a county basis. As these production levels represent the current demand of the country, it is assumed that all coal needed by the CBGTL process must be provided by additional production so that current usages of coal will not be affected. The estimated recoverable reserves from Table 15 of Energy Information Administration (2008a) are reported for each state and for each mine type (i.e., underground or surface). The recoverable reserves are decomposed into a county level by proportionally weighting the values based on the current production levels of the counties. Hence, for a given county with a known production and mine type, the estimated recoverable reserves for that county are calculated by using the estimated recoverable reserves for the same mine type in that state, and then multiplying that value by the ratio of the current production of the county mine divided by the total current production of all mines in the state of the same mine type. Given the estimated recoverable reserves for each county, the current lifespan of the mine is calculated by dividing the reserves by the current production level. If this value is less than 100 years, it is assumed that the production possible for CBGTL processes is only 20% of the current production. If greater than 100 years, than the production possible is equal to either (i) the additional production that would be required to have a 100 year lifespan, or (ii) 500% of the current production, whichever one has the lower value.

The minemouth cost of coal for each county initially utilizes information from Tables 28, 30, and 31 of Energy Information Administration (2008a). Table 30 gives the average price of coal

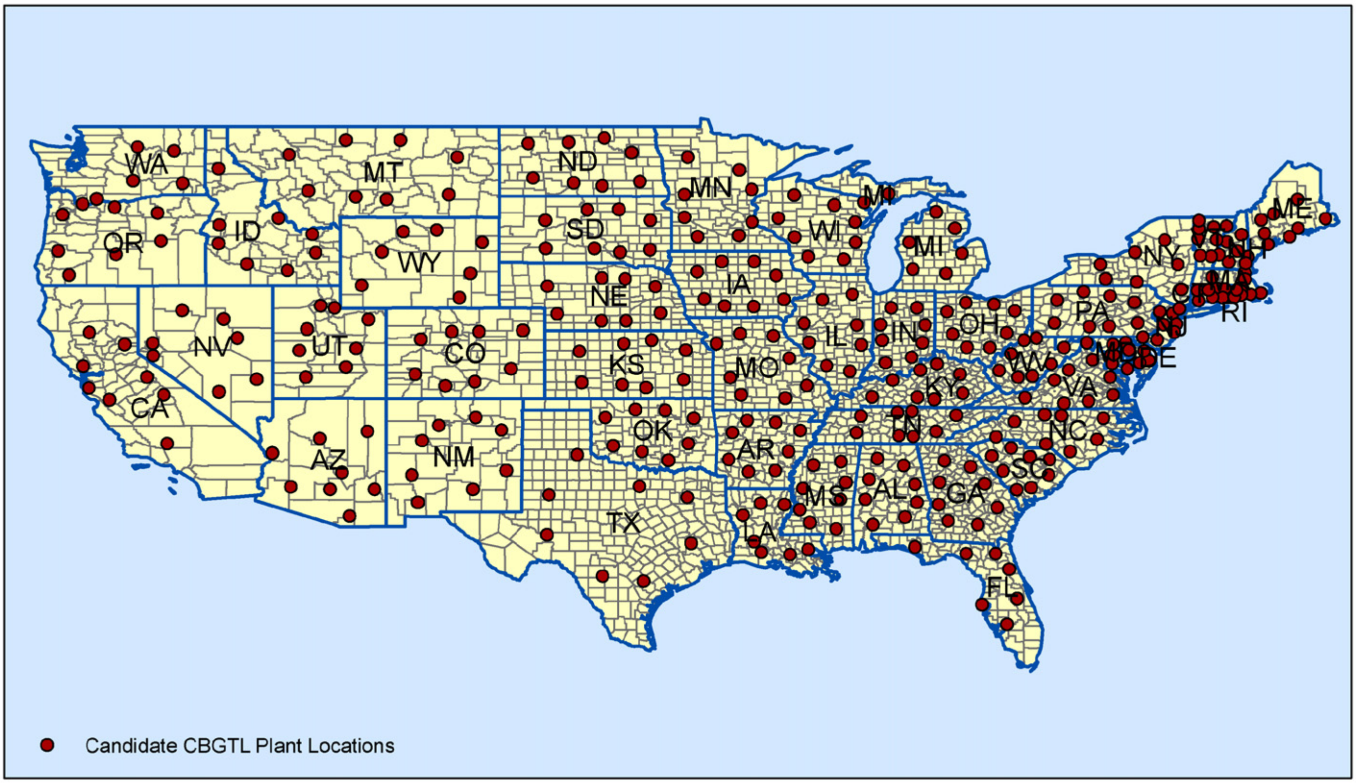

**Fig. 1.** Layout of the candidate locations for the hybrid CBGTL plants, which are located at the centers of state discretizations. Each state is divided into eight octants based on the state centroid. Several states that do not have enough number of counties are allowed to have less than eight discretizations.

for each county, Table 28 gives the average price per mine type for each state, and Table 31 gives the average price per coal type for each state. Cost data is taken from Table 30 when available and supplemented with the information from the coal type and the mine type in similar fashion to the determination of coal availabilities as described in the previous paragraph.

Though the Annual Coal Report (Energy Information Administration, 2008a) only gives reference to one type of bituminous coal, the NETL Quality Guidelines report (National Energy Technology Laboratory, 2004) recommends three distinct types, including high-volatile (HV), medium-volatile (MV), and low-volatile (LV) bituminous coal. To determine the resource locations of each category of the bituminous coal, a map on the coal reserves of the United States from the American Coal Foundation was used (American Coal Foundation, 2010). Based on this map, it is assumed that (i) VA, MD, and AR contain LV bituminous, (ii) WV counties including Lincoln, Mason, Randolph, Upshur, and Wayne contain MV bituminous while the remaining WV counties contain LV bituminous, (iii) AL, TN, PA, OH, and eastern KY contain MV bituminous, (iv) IL, IN, KS, MO, and western KY contain HV bituminous, and (v) WY, CO, YT, NM, and AZ are HV bituminous. The layout of coal sources in the United States is displayed in Fig. 2.

### 3.2. Biomass

Biomass feedstock data is largely categorized into two major groups: (a) agricultural residues and (b) forest residues. The agricultural residues include crop residues, perennial crops, grains for biofuels, animal waste, fats, and other feedstocks. This study will focus on crop residues, perennial crops, and grains. Animal manure and fats were not considered due to the sparse availability of data. Forest residues include logging residues, fuelwood, mill residues, and urban waste (Department of Energy and Department of Agriculture, 2005).

Per unit mass basis, biomass is one of the highest costing feedstock in the CBGTL network. Thus, the total amount spent on feedstock can be significantly reduced if the purchase cost of the biomass is reduced, which would require a reduction in nutrient replacement costs, harvesting and maintenance costs, and yield per acre. The National Research Council (National Academy of Sciences and National Academy of Engineering and National Research Council, 2009) has set “willingness-to-accept” prices for several biomass sources both currently and in 2020. If the target 2020 prices are able to be achieved, this will result in the decrease (prior to transportation) of 20% of the corn stover cost, 19% of the switchgrass cost, 14% of the forest residue cost, and 21% of the other crop cost (National Academy of Sciences and National Academy of Engineering and National Research Council, 2009).

#### 3.2.1. Agricultural residues (crops)

The National Agricultural Statistics Service (NASS) (2010) provides a database of all crop production throughout the country that is discretized on a county level. This data includes 59 types of crops that are produced by both irrigated and non-irrigated farming practices. To reduce the complexity of the crop types, a representative set of crops, including corn stover, sorghum, barley, oats, wheat, soybeans, rice, cotton, was chosen based on the Department of Agriculture (DOA) “Billion-Ton” study (Department of Energy and Department of Agriculture, 2005). All remaining crops were lumped into a generic residue category. All NASS production data are converted to mass units using the appropriate bushel size, if necessary. The production of a given crop was then related to the total amount of sustainable residue that can be harvested for the CBGTL process. The high crop yield increase with land use change study from Department of Energy and Department of Agriculture (2005) was used for each crop in the NASS database. It is assumed that (i) a portion of the recoverable corn grain (50% of baseline total or 20.25

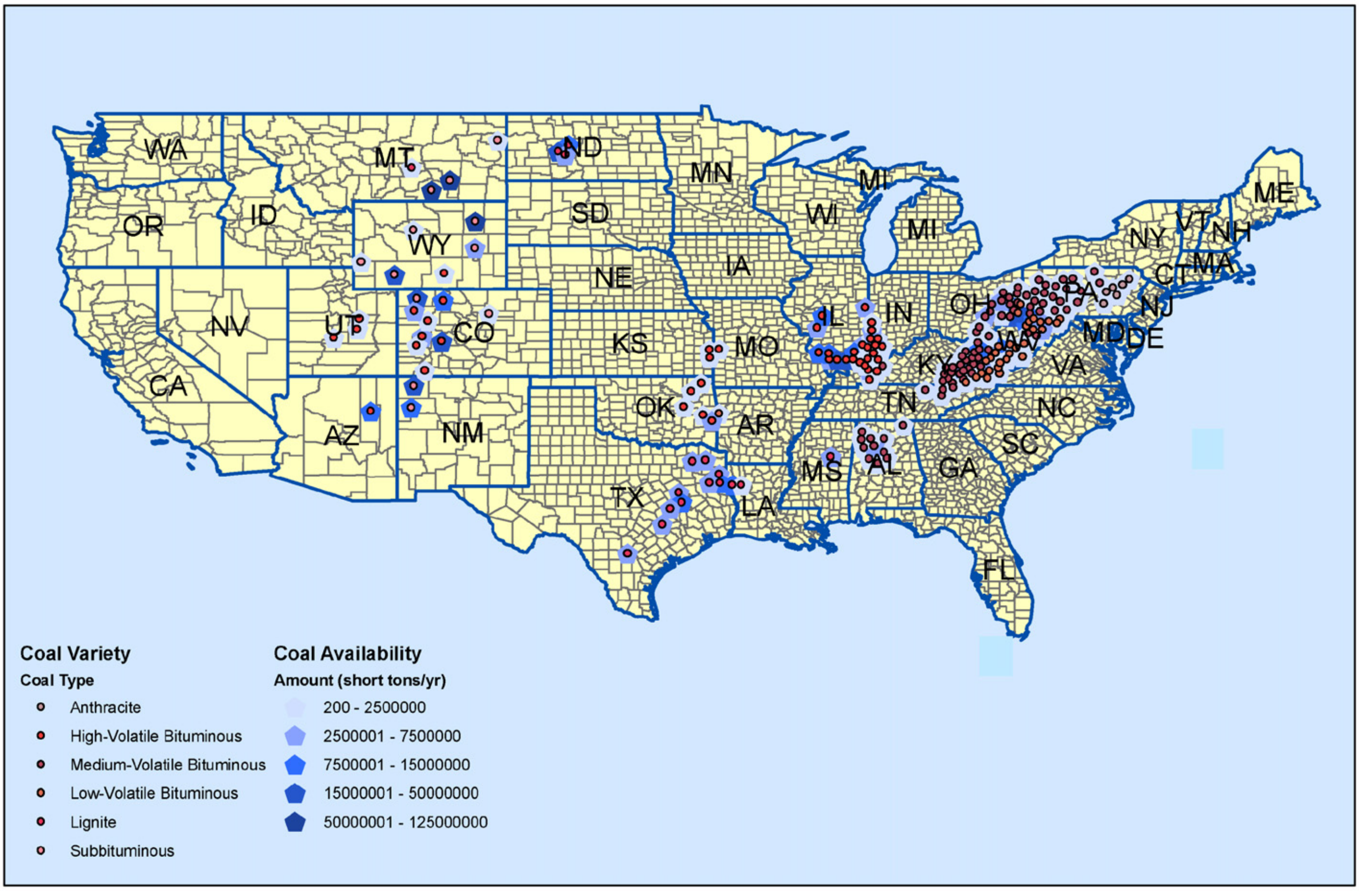

**Fig. 2.** The geographical layout of coal-producing locations within the United States and their respective production amounts. The variety of coal types produced in the United States is signified by the circles and the ranges of production amounts are represented by the pentagons, according to their respective proposed color schemes on the map.

million dry tons) is utilized for the production of ethanol and is unavailable to CBGTL processes, (ii) all crops listed as generic crops had the same ratio of sustainable residue yield to production yield, and (iii) the benefit from double cropping is proportionally assigned to each total value of crop residue based on the total sustainable amount for each crop.

Data from National Agricultural Statistics Service (2010) was largely discretized on an individual county level, but there are some cases where the production levels from multiple counties are grouped together based on their agricultural districts. In these instances, the biomass is assumed to be located at the centroid of the district, which is calculated as the geometric center of all counties associated with the district. If the sum of the production in all counties for a crop is less than the total production figure for the state, then the remaining production is assumed to be located at the centroid of the state, which is calculated as the geometric center of all counties associated with the state. Costing data for each crop is obtained by subtracting the cost of transportation from the 2008 baseline price presented in Table 2.5 of National Academy of Sciences and National Academy of Engineering and National Research Council (2009). Corn stover prices are used for the corn stover crop while the wheat straw prices are used for all other crops. The map of agricultural residues production in the United States is displayed in Fig. 3.

### 3.2.2. Agricultural residues (perennials)

All perennial crops are assumed to be switchgrass that is planted on available Conservation Reserve Program (CRP) land. The DOA Farm Service Agency lists the cumulative amount of CRP acreage by county (Department of Agriculture: Farm Service Agency, 2008). Using the total amount of perennials crops and CRP crops from Department of Energy and Department of Agriculture (2005) for the high crop yield with land use change study, the switchgrass potential production by state was decomposed over the country assuming that the potential for sustainable residue production is proportional to the available CRP acreage. Costing data for switchgrass is taken from baseline 2008 scenario (Table 2.5 of National Academy of Sciences and National Academy of Engineering and National Research Council, 2009) after subtracting the cost of transportation. The distribution of switchgrass production in the United States is shown in Fig. 4.

### 3.2.3. Forest residues

The total available forest residues for the CBGTL process are taken from Fig. 13 of Department of Energy and Department of Agriculture (2005) and include all unexploited residues and anticipated residues due to growth for logging residues, other removal residues, fuel treatments, fuelwood, forest products residues, and urban wood residues. The currently used fuelwood and urban wood residues are also assumed to be available while the existing residues that are currently used for forest products are assumed to be utilized for energy recovery or lignin production and are therefore unavailable for use as CBGTL feedstocks. Costing data for all forest residues is equal to the woody biomass 2008 baseline value from Table 2.5 of National Academy of Sciences and National Academy of Engineering and National Research Council (2009) after subtracting the cost of transportation.

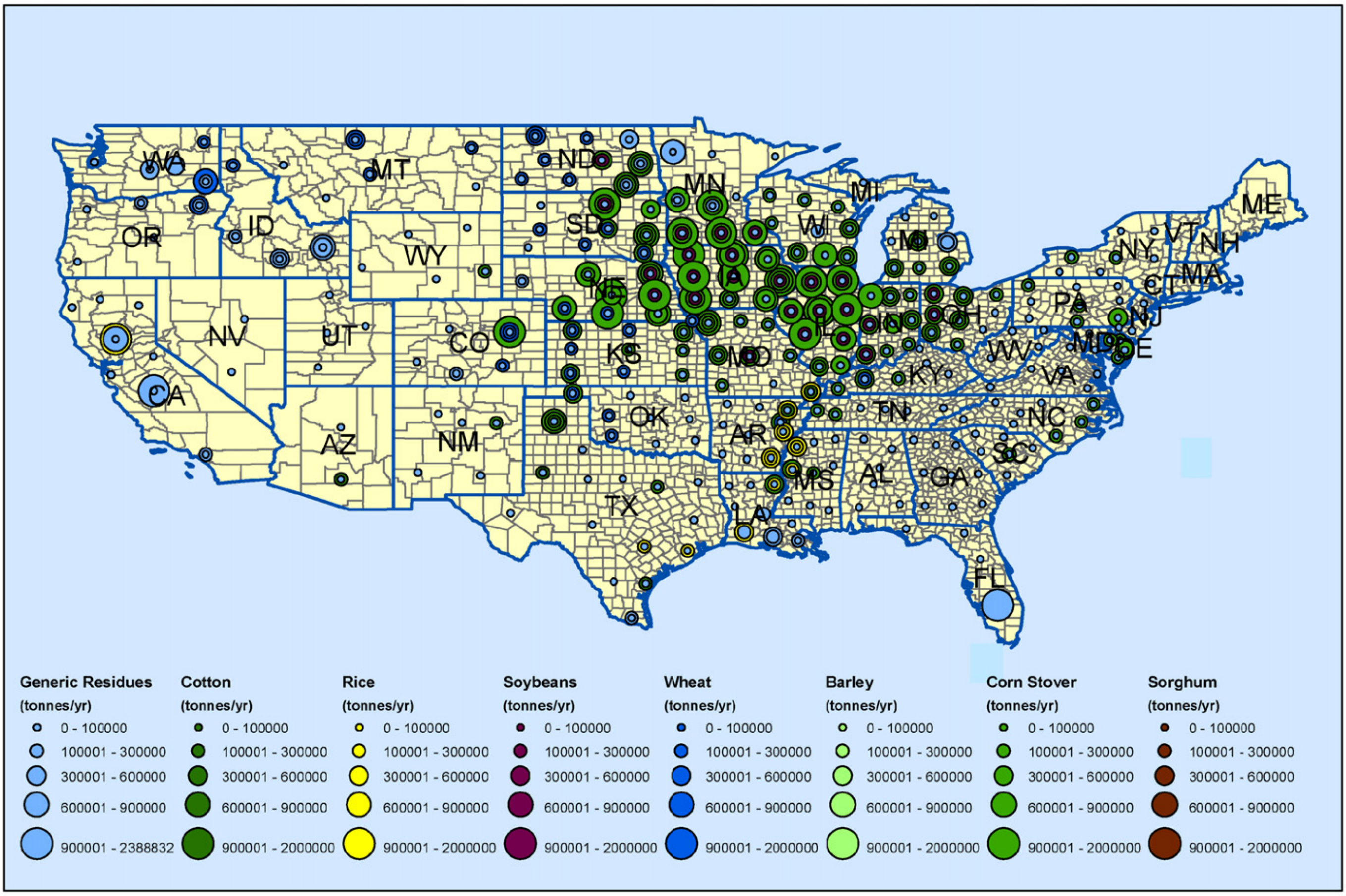

**Fig. 3.** The geographical layout of the availability of agricultural residues within the United States for the CBGTL supply chain network. The midwest region of the United States is shown to possess the highest availability of agricultural residues. Note that multiple types of agricultural residues may be present at a single location and their symbols may overlap in the displayed map.

The Federal Forest Service (FFS) (2008) provides information on the timber product output from all counties every five years, the most recent being 2006. Both hardwood and softwood data are reported for all types of timber removal, so four broad categories of timber residues were established: hardwood, softwood, hardwood mill residues, and softwood mill residues. Hardwood and softwood will be used to describe logging residues, other removal residues, fuel treatments, and fuelwood. The mill residues will be used to describe the residues generated from the forest products industry. The density of hardwood and softwood was initially calculated using Tables 11 and 12 of Department of Energy and Department of Agriculture (2005), resulting in 29.76 dry lbs/ft$^3$ for softwood and 31.33 dry lbs/ft$^3$ for hardwood. These density values were used to convert all volumetric data to the appropriate mass values.

Timber removals from Table C10 of Federal Forest Service (2008) includes the logging residues and other removal residues. These data were proportionally scaled up to the expected growth from Fig. 13 of Department of Energy and Department of Agriculture (2005) by assuming that the total logging residues includes the fuel treatments for both timberland and other forestland. The fuel treatment data was lumped with the logging residues due to the unavailability of the DOA Fuel Treatment Evaluator tool. Fuelwood from Table C5 of Federal Forest Service (2008) for each county was determined in a similar fashion for both hardwood and softwood. Mill residues for each county were extracted from Table C11 of Federal Forest Service (2008) and included filter, fuel, miscellaneous, and non-used byproducts. Each of these individual types of byproduct contains a distinct density calculated from Tables 11 and 12 of Department of Energy and Department of Agriculture (2005), which was used to convert the data to mass units. The total softwood and hardwood mill residues for each county was then summed over all byproducts and then scaled up so that the sum over the country was equal to the sum of the CBGTL residues available from the forest products industry.

To calculate the total amount of urban wood residues available, the State of Garbage in America study (Arsova, van Haaren, Goldstein, Kaufman, & Themelis, 2008) was utilized. This report gives the total amount of municipal solid waste that is landfilled, organics that are composted, and yard trimmings that are collected for the year. Data is available on a per state basis, so the urban waste feedstock is assumed to be located at the centroid of each state. The data for each state is summed and then normalized so that the total for the country is equal to the total urban wood residues from Fig. 13 of Department of Energy and Department of Agriculture (2005). The map of available forest residues for the CBGTL supply chain network is displayed in Fig. 5.

### 3.3. Natural gas

The EIA provides the natural gas production level, proved reserves, and wellhead prices on a per state basis. The amount of natural gas available for the potential CBGTL plants is obtained by calculating the average annual technically recoverable natural gas, including conventional and unconventional gas recovery (i.e., natural gas from tight gas basins, shale basins, and coalbed methane basins) that is not already in use by current industries and energy

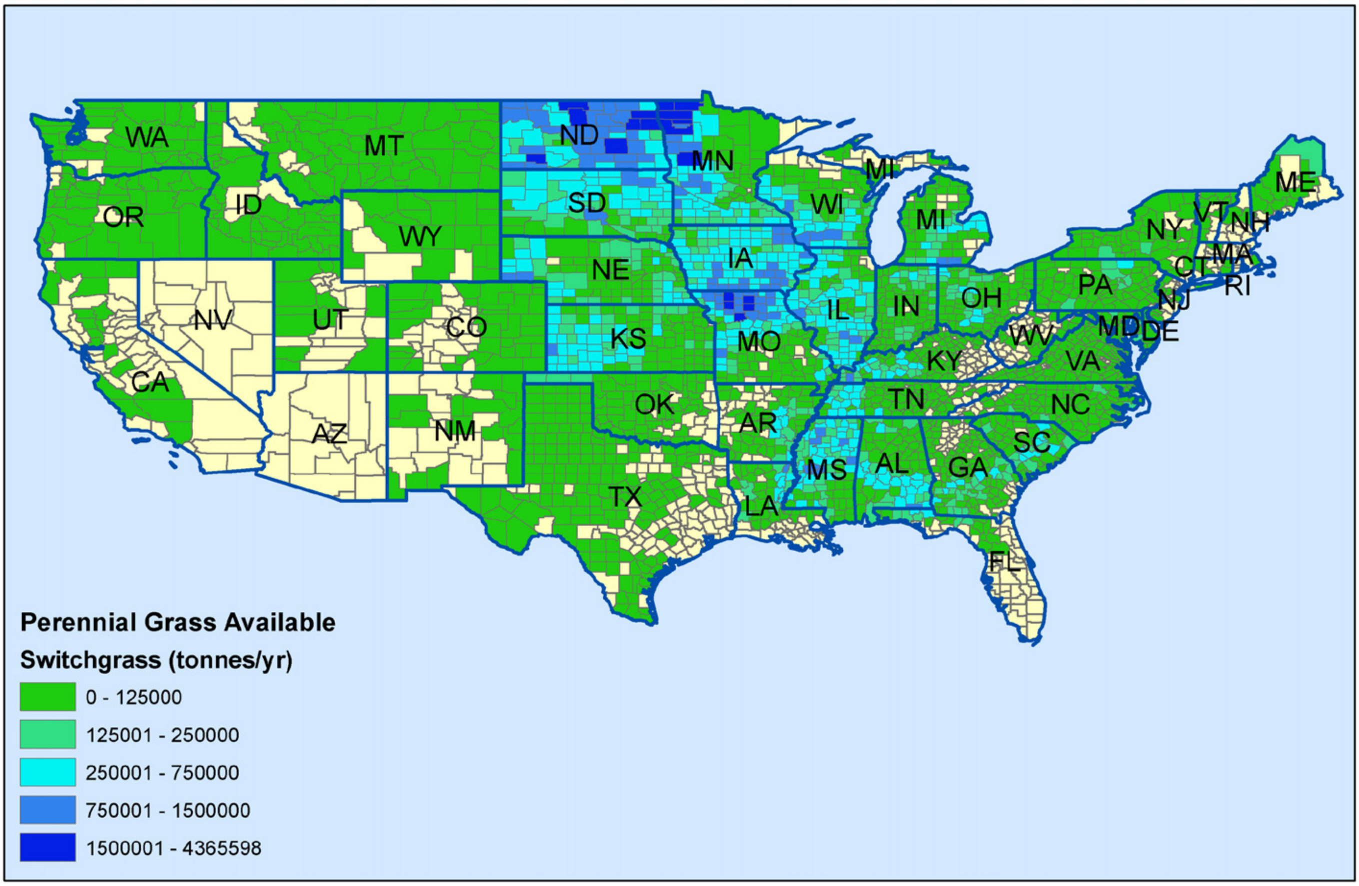

**Fig. 4.** The geographical layout of switchgrass production based on Conservative Reserve Program (CRP) land acreage within the United States.

infrastructure. We assume that the entire technically recoverable amount will be exhausted in 50 years by the production for current industries and for the CBGTL process. The EIA estimates that the unproved reserves of natural gas in the United States is about seven times larger than the current proved reserves. Based on this factor, the unproved reserves is calculated and the total production rate consumed by existing industries for the next 50 years are subtracted from the total amount, based on the assumption that the production amounts are entirely consumed by current industries. This total production is calculated based on the annual projected increase of 0.9% (Energy Information Administration, 2010d). The locations of natural gas sources are assumed to be at the centroid of the states that have natural gas wells in their regions. We assume that the state centroid is a hub of natural gas gathering pipelines from the various wells, and the CBGTL network will purchase and transport natural gas from these hubs. The map of natural gas availability in the United States is shown in Fig. 6.

### 3.4. Hydrogen

On a per unit mass basis, hydrogen is the most expensive feedstock required for the CBGTL process. The largest production of hydrogen today comes from the steam reforming of methane, using natural gas as feedstocks (National Research Council, 2004). However, coal and biomass can also be used as feedstocks via gasification and synthetic gas separation technologies. Alternatively, hydrogen can also be produced via electrolysis by using water as feedstock and electricity. However, with the current cost of electricity and the capital cost of electrolyzers, the non-carbon-based option is not economically attractive for large scale hydrogen production. Current hydrogen production prices from coal, biomass, and natural gas feedstock range from about $1.00/kg to $1.25/kg (Chiesa, Consonni, Kreutz, & Williams, 2005; Larson et al., 2009; National Research Council, 2004) while those from non-carbon sources are typically between $2.00/kg and $10.00/kg and are strongly dependent on the cost of electricity needed to power the electrolyzers (National Research Council, 2004).

The effects of hydrogen prices on the topology of the CBGTL network are studied in two different case studies in Section 7. Hydrogen is supplied at fixed prices in case study 1 assuming that it is produced by steam reforming of methane. In case study 2, the feedstock availabilities for carbon-based technology options are taken into account. Hydrogen can be produced via coal gasification, biomass gasification, or steam reforming of methane at the CBGTL site. The investment costs of these systems are included in the overall cost of the network, scaled appropriately with the amount of hydrogen produced by the system.

## 4. Demand amount and location

The demand of petroleum based products used for transportation is extracted from the EIA State Energy Data System 2008 report (Energy Information Administration, 2008c). Though the exhaustive list of products includes aviation gasoline, distillate fuel oil, jet fuel, liquid petroleum gas (LPG), lubricants, motor gasoline, and residual fuel oil, a large majority of the products is represented by distillate fuel oil (2841 thousand barrels per day (TBD); 20.7%), jet fuel (1543 TBD; 11.2%), and motor gasoline (8859 TBD; 64.4%) (Energy Information Administration, 2008c). Therefore, each CBGTL facility is designed to produce each of these three fuels in the same

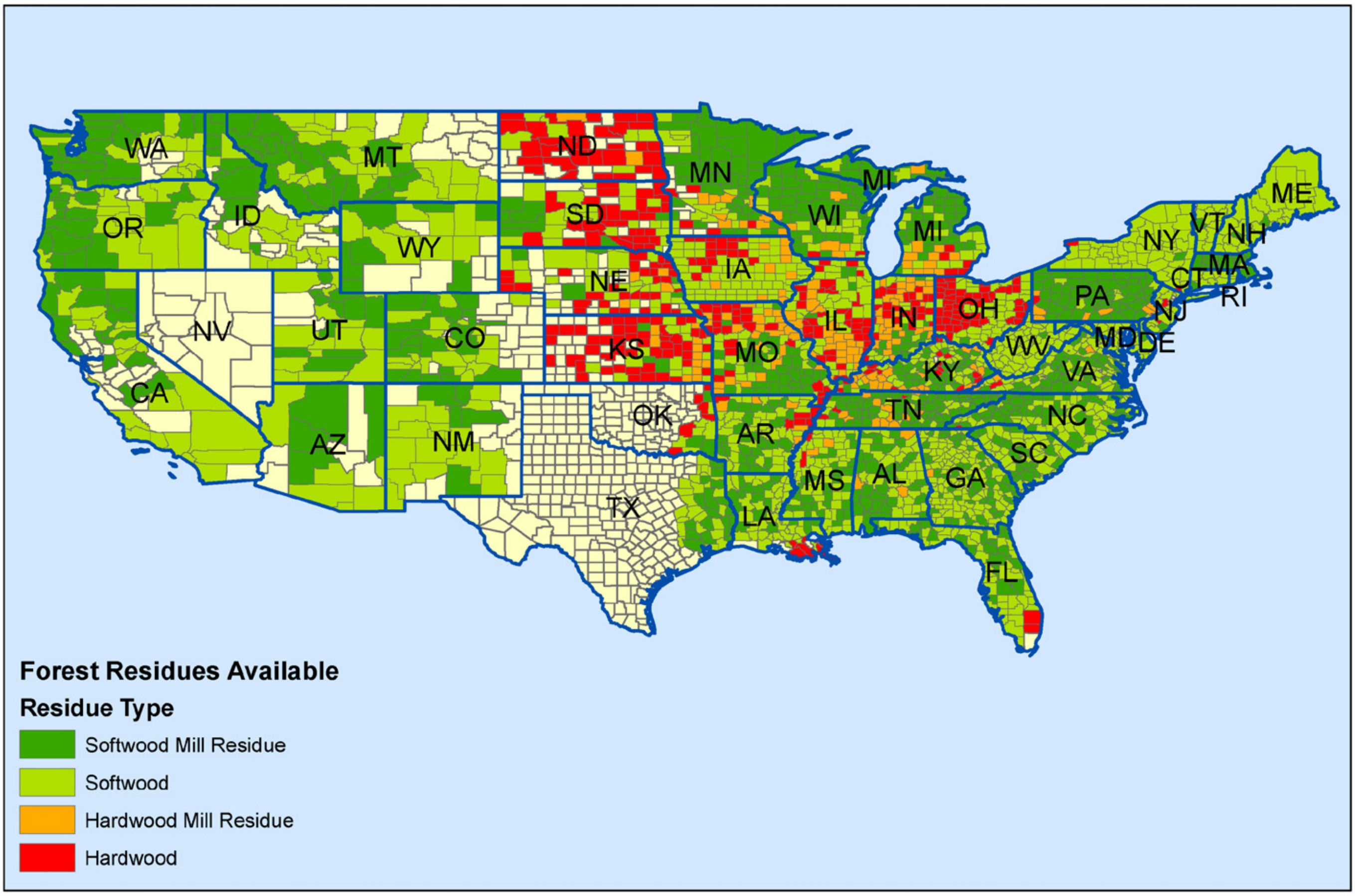

**Fig. 5.** The geographical layout of forest residues available for the CBGTL supply chain network.

ratio required to satisfy the entire U.S. 2008 demand. All demand data are available on a statewide basis, so a discretization of the demand amounts to a county level was not possible. It is assumed that the final demand location for each state is the centroid of the state, as calculated from the corresponding county centroid of the state. The cost to deliver the products to the centroid of the state will therefore be an estimate of the average cost to deliver to each individual county.

## 5. Modes of transportation

Feedstock will be transported from their locations to the CBGTL plant locations, while the fuel products will be transported from the CBGTL plant locations to their demand sites. Coal, biomass, and natural gas are assumed to use one mode of transportation at each instance, either by truck, rail, or pipeline, depending on the type of feedstock being transported (see Table 5). Transportation of the products, on the other hand, will utilize truck, pipeline, or barge and can use either one mode (truck or pipeline only) or two modes (barge along with truck or pipeline) of transportation.

**Table 5**
Allowed modes of transportation for each feedstock and product and their respective cost limitation. The cost limitation represent the worst allowable transportation cost of each commodity.

| Feedstock/product | Allowed modes of transportation | Transportation cost limitation ($/GJ delivered) |
|---|---|---|
| Coal | Truck, railroad | $10 |
| Biomass | Truck | $2 |
| Natural gas | Truck, pipeline | $10 |
| Fuel products | Truck, pipeline, barge | $10 |

Transportation costs via truck, rail, or barge are calculated using Eq. (15), which is based on a distance fixed cost (*DFC*), a distance variable cost (*DVC*), the distance traveled (*Distance*), and a distance multiplier (*DM*). For truck and rail transport, *Distance* is simply the straight line distance between the two points calculated from the latitude and longitude. To account for path curvatures, the distance is increased by a factor of *DM*. For truck, *DM* is equal to 1.1 while for rail, *DM* is equal to 1.05. The barge distances used are exact and thus *DM* is equal to 1. Transportation via pipeline is given as a cost per unit quantity of shipped material directly from the individual pipeline companies:

$$Cost = DFC + DVC \cdot Distance \cdot DM \qquad (15)$$

To prevent large number of combinations between the origin and destination points, we impose a cost limitation on the transportation of feedstocks and products. That is, for a given pair of origin and destination points, if the transportation cost exceeds the predetermined limits, the match is not allowed. The allowable limits of transportation cost are included in Table 5.

### 5.1. Truck

The *DFC* and *DVC* parameters for transportation via truck are given in Table 6 for each component in the energy supply chain network (Searchy, Flynn, Ghafoori, & Kumar, 2007). It is assumed that transportation via truck will utilize the current roadway network without the need for highway expansion. We note that our assumptions on the distances traveled by truck transportation differ from

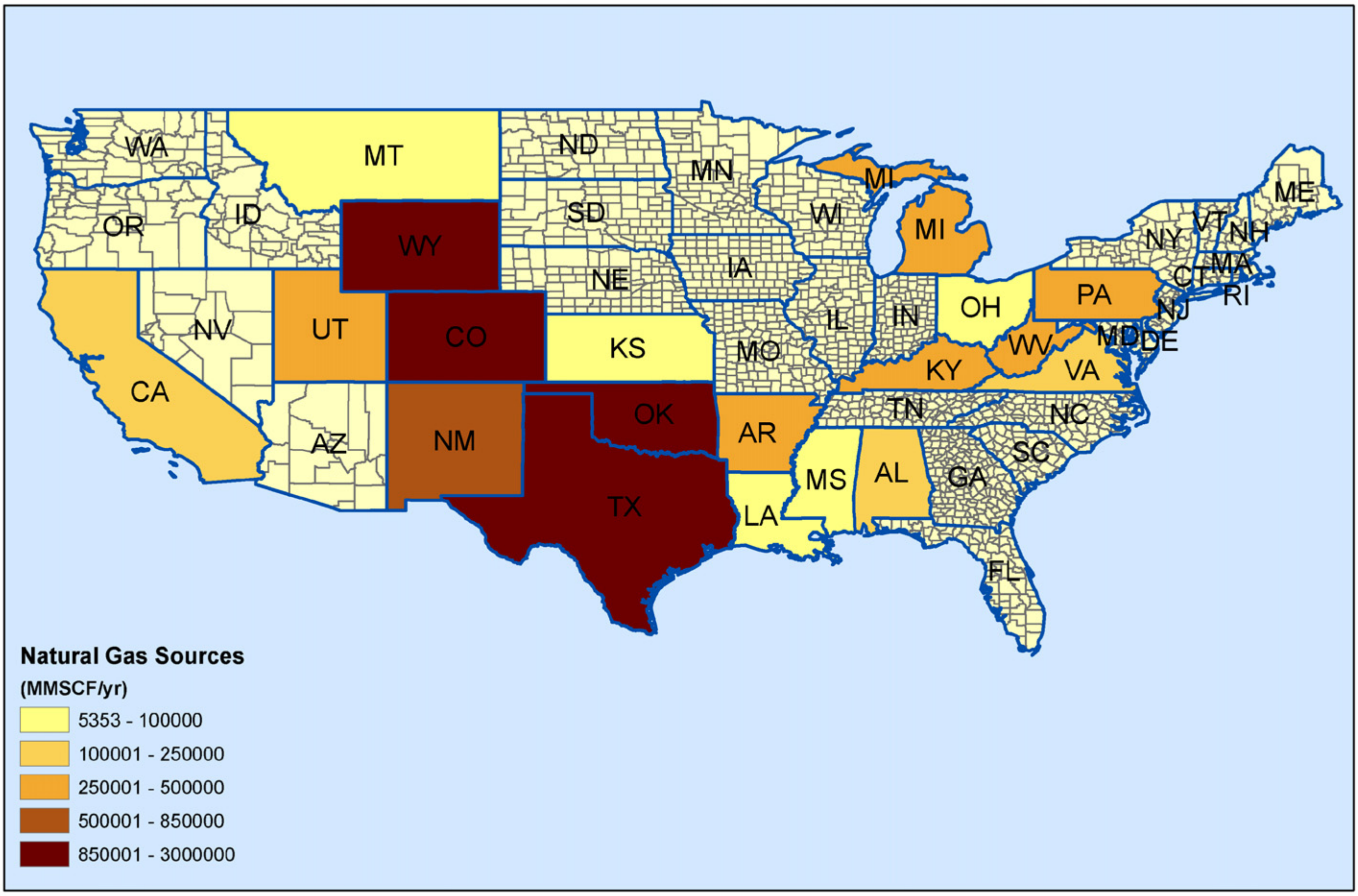

**Fig. 6.** The geographical layout of natural gas resources for the CBGTL supply chain network. The ranges of each state's production amounts are displayed according to the color scheme proposed on the map.

the ones used in the GREET model. In the GREET model, each commodity has an associated distance number for truck transportation (see Appendix A). In our mathematical model, there is no limitation on the distance traveled by any commodity by truck. The only limitation imposed for transportation of feedstock and products is in the transportation cost of delivered feedstock and products as mentioned before. This assumption follows for rail, pipeline, and barge as well.

Note that the biomass cost parameters in Table 6 correspond to feedstock that is harvested without further pretreatment. Each biomass feedstock is assumed to be fully pretreated on site at the CBGTL refinery. It is possible to reduce the feedstock costs for biomass using a pretreatment process (e.g., torrefaction) on the feedstock growth site at the expense of some levelized investment cost of the pretreatment facility. Such pretreatment facilities that may improve the biomass properties can be easily incorporated in the proposed approach, and will be the study of a future investigation.

### 5.2. *Railroad*

Although biomass and the liquid products can be transported by rail, this study solely focuses on the rail transportation of coal due to the extensive network currently available for the shipping of coal via rail to power plants across the country. The Surface Transportation Board produces a public use waybill (Surface Transportation Board, 2008) each year with the details of all rail shipments across the country from carriers above a certain minimum threshold capacity. The public waybill data uses business economic areas (BEAs) to mark the starting and ending points for a delivery. To extract *DFC* and *DVC* for coal shipments between a given pair of BEA codes, the cost, weight, and distance data for all samples that have a delivery between the two codes are used in a linear regression model. As each county in the country can be mapped to a specific BEA code, the values of *DFC* and *DVC* between any two counties is assumed to be equal to the values for the BEA codes that represent the counties.

**Table 6**
Truck cost parameters, including the distance fixed cost (*DFC*) and the distance variable cost (*DVC*).

| Feedstock/product | Distance fixed cost (*DFC*) | Unit | Distance variable cost (*DVC*) | Unit | Ref. |
|---|---|---|---|---|---|
| Coal | 6.98 | $/short ton | 0.286 | $/short ton-mi | Searchy et al. (2007) |
| Biomass – crop residue | 4.839 | $/tonne | 0.213 | $/tonne-mi | Searchy et al. (2007) |
| Biomass – forest residue | 3.318 | $/tonne | 0.124 | $/tonne-mi | Searchy et al. (2007) |
| Natural gas | 25225.18 | $/MSCF | 151.92 | $/MSCF-mi | – |
| Fuel products | 3.318 | $/bbl | 0.124 | $/bbl | Searchy et al. (2007) |

### 5.3. *Pipeline*

Transportation of both natural gas and the liquid products via pipeline will build upon the current pipeline infrastructure for each component. Natural gas will be transported only via pipelines, while liquid fuel products can either be transported via pipelines or a combination of pipelines, trucks, and barges.

#### 5.3.1. *Natural gas*

The current natural gas pipeline infrastructure consists of intrastate and interstate pipelines. From the database provided by the EIA (Energy Information Administration, 2010a), we identified a list of states that currently have intrastate pipeline structures. The cost parameters associated with the use of these pipelines are the state transmission and distribution prices provided on the EIA website. For interstate natural gas transmission, we utilized a EIA database that reports the starting and ending locations of interstate pipelines along with their capacities and average daily flows. The available capacities for the CBGTL process are the portions that are not used by current flows. The usage costs of these pipelines are obtained from the informational postings of the associated pipeline companies.

#### 5.3.2. *Products*

Transportation of products from plant locations to demand locations via pipeline builds upon the current pipeline infrastructure for petroleum products. Information on pipeline origin and end locations, as well as their usage fees, are obtained from the informational postings of 10 largest pipeline companies in the United States. It is important to note that several of the largest pipelines are designed to transport the products from locations which produce or import the largest quantities of products to other demand locations. As such, the southern part of the United States, including Texas and Louisiana, contain the starting points for many pipelines. However, these states may not prove to be optimal locations of facilities that utilize biomass, coal, and natural gas due to the feedstock transportation costs. Thus, it is crucial that expansion of the products pipeline network is considered via an extension of the current pipeline network.

#### 5.3.3. *Expansion of current network*

Expansion of the current natural gas and products pipeline networks is a likely prerequisite for implementing a CBGTL network for the country. The increased amount of United States natural gas demand can be accompanied by the remaining capacity of the current pipeline network, but extension of the pipeline will be required to connect current pipeline outlets to the CBGTL facility. Additionally, the presence of CBGTL plants in regions that currently have little products pipeline infrastructure will require either construction of new pipelines or extension of previous lines.

Let the total number of current natural gas pipelines be $N_{Pipe}^{NG}$ and the total number of current products pipelines be $N_{Pipe}^{Prod}$. Given a CBGTL facility location, *facility*, and a natural gas source county, *county*, the natural gas may flow through each of the $N_{Pipe}^{NG}$ pipelines by extending the pipeline from (a) the *county* to the pipeline inlet and from (b) the pipeline outlet to *facility*. A pipeline extension (and therefore a connection from *county* to *facility* using that pipeline) is considered infeasible if the additional extension pipeline length is longer than the length between *county* and *facility*. The cost associated with expanding the pipeline is calculated using the cost per unit of natural gas associated with that specific line. This cost is first divided by the length of the pipeline and then multiplied by the total length of the pipeline plus extension.

The expansion of the products' pipelines is determined in a similar manner. However, the possibility of developing a completely new pipeline between a facility and a demand location is also considered. That is, for any given CBGTL facility, *facility*, and demand location, *county*, products may flow through each of the $N_{Pipe}^{Prod}$ pipelines by extending the pipeline or they may flow through a completely new pipeline beginning at *facility* and ending at *county*. Pipelines are considered infeasible if conditions similar to (a) or (b) above are satisfied. To incorporate multiple modes of transportation, this approach is also utilized between *facility* and any oil seaport, *port*, by considering all possible products pipelines between *facility* and *port* or developing a new pipeline between *facility* and *port*. To deliver products to the final demand location, the same method is also applied between all pairs of *port* and *county*. Note that when extending a specific pipeline, the cost of expansion is calculated using the current cost per unit product associated with that pipeline. If a new pipeline is to be constructed, the cost per unit product used is the average of all pipelines.

### 5.4. *Barge*

The gasoline, diesel, and kerosene products can be transported by barge as part of a bimodal system. A comprehensive list of United States oil seaports is obtained from the list of 2008 United States petroleum based imports from the EIA (Energy Information Administration, 2008b). A total of 167 active sites were extracted and then ranked according to the total quantity of all imports received for the year. Port locations in the Virgin Islands and Puerto Rico were excluded since these regions were not considered in the energy supply chain model.

The ports were mapped to their corresponding longitude and latitude specifications obtained from the World Port Source (2010). All import locations in MT, ND, and CO were omitted since no record of a port could be found. A list of 50 ports was then extracted consisting of the 49 remaining highest ranked ports and 1 port in Anchorage, AK to provide an available connection to Alaska for the model solution. Port-to-port distances are extracted from an online World Ports Distances calculator (Distances.com, 2010). All ports that do not have an entry in the World Ports Distances database are listed in Table 7, along with their respective reference ports (closest port location with available distance information). The adjustment distance is the known distance in nautical miles between the unaccounted ports and their corresponding reference ports. This adjustment factor is used to infer the distances for the unaccounted ports. Specific assumptions made for each ports can also be found in Table 7.

## 6. Energy supply chain model

Given (i) the locations of biomass, coal, and natural gas feedstocks and their respective availabilities and costs, (ii) the locations and demands of products, (iii) the investment costs associated with the CBGTL plants, and (iv) the modes of transportation available to feedstock and product delivery, we seek to identify the optimal locations of the CBGTL plants throughout the United States that minimize the overall cost of the energy supply chain network. A mixed-integer linear optimization (MILP) model was formulated to identify the topology of the CBGTL supply chain network by introducing binary variables to represent the discrete decisions on (a) plant location, (b) plant size selection, and (c) feedstock type for each candidate CBGTL plant. A fixed grid of points was chosen for the plant locations by discretizing each state in the United States into octants and assuming that the centroid of each octant is a candidate location for a CBGTL plant (see Section 2.2). Each CBGTL plant must use exactly one type of coal and one type of biomass with the proportion of each feedstock determined *a priori* from a preliminary life cycle analysis that aims for a 50% reduction in GHG emissions from current petroleum based processes. Continuous variables

**Table 7**
Port distances assumptions.

| Unaccounted ports | Reference ports | Adjustment distance in nautical miles | Assumptions |
|---|---|---|---|
| Newark, NJ | New York, NY | 12 | Distances to and from Newark, NJ are adjusted accordingly for eastern and western ports. |
| Morgan City, LA<br>Pasagoula, MA | Port Arthur, TX | 0 | Distances to Gulf Coast ports are taken from reference.<br>Distances to other ports take the values of distances from Port Arthur, TX and adjusting based on the distance to the Straight of Florida for eastern ports and the Yucatan channel for western ports. |
| Richmond, CA | San Francisco, CA | 11 | Add 11 nautical miles to all San Francisco, CA distances, except for Martinez, CA (subtract 11 nautical miles). |
| Bellingham, WA | Anacortes, WA | 17 | Add 17 nautical miles to all Anacortes, WA distances. |
| Port Huron, MI<br>Sault Ste. Marie, MI | Toledo, OH | 0 | Distances to Great Lakes ports are taken from reference.<br>Distances to other ports take the values of distances from Toledo, OH, adjusting based on the distance to Montreal, Quebec. |
| Gramercy, LA | St. Rose, LA | 30 | Add 30 nautical miles to all St. Rose, LA distances, except for Baton Rouge, LA (subtract 30 nautical miles). |
| Carquinez Strait, CA | Martinez, CA | 5 | Subtract 5 nautical miles from all Martinez, CA distances. |

are used in the model to represent the flow of feedstocks and products throughout the country. The following sections describe the developed mathematical model in detail. Descriptions of all indices, sets, parameters, and variables in the model can be found in Appendix B.

### 6.1. Sets

Given a political map of the United States, the country is discretized into a set of states $S$ and counties $C$:

$s \in S = \{\text{all United States states}\}$
$c \in C = \{\text{all United States counties}\}$

The elements of these sets are based on the Federal Information Processing Standard (FIPS) codes which designate all states with two-digit numbers and all counties as five-digit numbers.

All carbon-based feedstocks are partitioned into sets for forest biomass residues ($F^{B-fr}$), agricultural biomass residues ($F^{B-cr}$), coal ($F^C$), and natural gas ($F^N$), defined as:

$F^{B-fr} = \{\text{ urban wood waste, hardwood, softwood, hardmill waste, softmill waste }\}$
$F^{B-cr} = \{\text{ corn stover, oats, wheat, barley, switchgrass, sorghum, rice, cotton, soybeans, generic residue }\}$
$F^C = \{\text{ HV bituminous, MV bituminous, LV bituminous, subbituminous, lignite, anthracite }\}$
$F^G = \{\text{ natural gas }\}$

A set of all feedstocks, $F$, is generated as the union of the above four sets and a set of all biomass feedstocks, $F^B$, is generated from the union of the forest and agricultural residues:

$f \in F = F^{B-fr} \cup F^{B-cr} \cup F^C \cup F^N$
$f \in F^B = F^{B-fr} \cup F^{B-cr}$

Each CBGTL facility must use exactly one type of biomass, coal, and natural gas. The set $FC$ is defined by enumerating all possible combinations of feed triplets:

$$FC = \{(f, f', f'') | f \in F^C, f' \in F^B, f'' \in F^G\}$$

The set of products, $P$, represents the three liquid transportation fuels that have the highest demand throughout the country:

$$p \in P = \{\text{gasoline, diesel, kerosene}\}$$

Given the feedstock availability ($FA_{f,c}$) and product demand ($DM_{p,c}$) throughout the country, the set of all feedstock-county pairs ($C_F$) and product-county pairs ($C_P$) is defined:

$C_F = \{(f, c) | (f, c) \in F \times C, FA_{f,c} > 0\}$
$C_P = \{(p, c) | (p, c) \in P \times C, DM_{p,c} > 0\}$

The feedstocks and products can be transported via various modes of transportation ($M$) including truck, rail, pipeline, and barge. The biomass and natural gas will only be available by truck or pipeline, respectively, while the coal can be delivered by truck or rail. The products can be delivered by truck, pipeline, or barge. These combinations are represented as a set of all feedstock-mode pairs ($M_F$) and product-mode pairs ($M_P$). For pipeline transport of natural gas, there are several current lines with known capacity throughout the country ($M^G_{Pipe}$). The natural gas can be transported in one of these lines by expanding the line to travel to the CBGTL facility or an entirely new line can be constructed. A set of pipelines for product transportation ($M^P_{Pipe}$) is also given, and products can be transported via one of these lines or through a new line. The use of barge transport for the products is part of a bimodal system where the products are first transported to a port via pipeline, then shipped to another port, and finally delivered to the facility using another pipeline. The locations for barge transport ($R$) consists of fifty United States ports that were chosen based on their current liquid fuels capacity:

$m \in M = \{\text{truck, rail, pipeline, barge}\}$
$M_F = \{(f, m) \in F^B \times \text{truck} \cup F^C \times \{\text{truck, rail}\} \cup F^G \times \text{pipeline}\}$
$M_P = \{(p, m) \in P \times \{\text{pipeline, truck, barge}\}\}$
$r \in R = \{\text{50 United States ports with high liquid fuels capacity}\}$

The set of plant sizes, $T$, consists of small, medium, and large plants with production capacities of 10,000 BPD, 50,000 BPD, and 200,000 BPD, respectively:

$$t \in T = \{\text{small, medium, large}\}$$

The set $L$ contains all possible locations for the CBGTL plants, and is obtained from discretizing the United States regions using the method described in Section 2.2:

$$l \in L = \{\text{state discretizations}\}$$

Give the sets of feedstock combinations ($FC$), plant sizes ($T$), and plant locations ($L$), the enumerated set of all possible CBGTL facilities ($EFL$) is constructed:

$$EFL = \{(f, f', f'', t, l) \in FC \times T \times L\}$$

The mathematical model will consider a binary variable for each distinct facility location, so the computational complexity will increase dramatically as the number of plant locations increases. However, several elements in *EFL* will correspond to facilities that are located far from the counties that produce the feedstocks needed as input to the plant. A set of all quadruplets (*FT*) is created by listing the counties $c$ that can deliver a feedstock $f$ via transportation mode $m$ to facility location $l$ for an amount that is cheaper than the maximum cost $MaxCost_f^{FE}$ for the feedstock on an energy basis. That is, if the \$/GJ cost of feedstock transportation to a facility exceeds the maximum threshold, then the transportation of the feedstock from that county is not considered for that mode. A similar set of quadruplets (*PT*) is created for product transportation. Due to the high number of biomass feedstock counties, the choice of $MaxCost_f^{FE}$ for the biomass will have the greatest effect on the model solution time. In this study, the maximum was set to \$2/GJ for biomass and \$10/GJ for coal, natural gas, and the products (see Table 5). A smaller maximum can be used for the non-biomass materials, but it does not have a marked effect on the solution time of the model. Note that the delivery cost for a feedstock on an energy basis is calculated from the cost per unit mass times the feedstock lower heating value:

$$FT = \{(f, c, l, m) | (p, c) \in C_F,\ l \in L,\ (f, m) \in M_F,\ Cost^{FE}_{p,c,l,m} \le MaxCost^{FE}_f\}$$

$$PT = \{(p, l, c, m) | (p, c) \in C_P,\ l \in L,\ (p, m) \in M_P,\ Cost^{PE}_{p,c,l,m} \le MaxCost^{PE}_p\}$$

Given the set *FT*, a reduced facility list, *FL*, can be constructed by viewing the feedstock availability for a given element in *EFL*. If enough feedstock is available to satisfy the CBGTL plant requirement for each of the three inputs, then this facility is added to the set *FL*. The authors note that while the use of an upper bound for feedstock transportation cost will potentially eliminate feasible solutions from the mathematical model, the problem begins to become increasingly complex as the values for $MaxCost_f^{FE}$ (specifically, the biomass feedstocks) increase. It was found that \$2/GJ for biomass gave an appropriate balance between model tractability and solution quality. That is, using a value of \$3/GJ led to a solution within 0.5% of the original with a solution time increasing by 5–6 fold (about 1 day to about 1 week).

### 6.2. Variables

We use continuous variables to represent the levelized investment cost for a CBGTL plant ($Cost_l^I$), the hydrogen cost ($Cost_l^H$), the electricity cost ($Cost_l^E$), the flow of feedstock from the producing locations to the plant facility ($x_{f,c,l,m}$), the required flow rate of feedstocks to a plant facility ($FR_{f,l}$), and the flow of products transported from the plant facility to the demand locations ($z_{p,l,c,m}$). Binary variables ($y_{f,f',f'',l,t}$) are introduced to represent the existence of a specific CBGTL plant type (i.e., a specific combination of plant size and coal, biomass, and natural gas feedstock types). The complete variable list is presented below.

*Continuous variables*

$Cost_l^I$ : Levelized investment cost of facility $l$.
$Cost_l^H$ : Hydrogen cost of facility $l$.
$Cost_l^E$ : Electricity cost of facility $l$.
$x_{f,c,l,m}$ : Flow of feedstock $f$ from county $c$ to facility $l$ using transportation mode $m$.
$z_{p,l,c,m}$ : Flow of product $p$ from facility $l$ to county $c$ using transportation mode $m$.
$FR_{f,l}$ : Amount of feedstock $f$ requirement at facility $l$.

*Binary variables*

$y_{f,f',f'',l,t}$ : Existence of a CBGTL plant at location $l$ with feed combination $(f, f', f'') \in FC$ and size $t$. (15)

### 6.3. Constraints

The model constraints are classified into two major categories, namely (i) constraints on the logical existence of CBGTL plants, and (ii) feedstock and product flow constraints. The first category consists of equations that govern the existence of the CBGTL plants allowed in the network. Each facility location (i.e., the centroid of each state octant) is allowed to have at most one candidate CBGTL plant. Lower and upper limits on the number of small, medium, and large CBGTL plants across the United States are imposed. Feedstock requirements, production capacity, investment cost, hydrogen cost, and electrity cost are set for each facility location based on the candidate CBGTL plants. The second category of constraints relate the feedstock flow variables to their respective availabilities by county and the required flow rate amounts by facility. Likewise, the product flow variables are related to the facility production and the county demand. The required amounts of various inputs to the CBGTL process are extracted from the Aspen Plus simulation results. An objective function is used to minimize the overall cost associated with facility investment, feedstock purchase and transportation, and product transportation.

#### 6.3.1. Candidate CBGTL plant constraints

The following constraints will enforce the logical use of CBGTL facilities throughout the country. First, there should only be at most one facility selected at each location (Eq. (16)). Additionally, an upper bound is placed on the total number of facilities (Eq. (17)) and the number of facilities of a given size (Eq. (18)). A minimum number of facilities of each size is also enforced using Eq. (19). In this study, $N = 250$, $N_t^{\max} = 150\,\forall t$, and $N_t^{\min} = 10\,\forall t$:

$$\sum_{(f,f',f'',t,l) \in FL} y_{f,f',f'',t,l} \le 1 \quad \forall l \in L \tag{16}$$

$$\sum_{(f,f',f'',t,l) \in FL} y_{f,f',f'',l,t} \le N \tag{17}$$

$$\sum_{(f,f',f'',t,l) \in FL} y_{f,f',f'',l,t} \le N_t^{\max} \quad \forall t \in T \tag{18}$$

$$\sum_{(f,f',f'',t,l) \in FL} y_{f,f',f'',l,t} \ge N_t^{\min} \quad \forall t \in T \tag{19}$$

The levelized investment cost of a facilitiy location ($Cost_l^I$) is determined from the levelized costs of the candidate facilities ($LC_{f,f',f'',t}$) using Eq. (20). Similarly, the cost of hydrogen ($Cost_l^H$) and electricity ($Cost_l^E$) is determined using Eqs. (21) and (22):

$$\sum_{(f,f',f'',t,l) \in FL} y_{f,f',f'',l,t} \cdot LC_{f,f',f'',t} = Cost_l^I \quad \forall l \in L \tag{20}$$

$$\sum_{(f,f',f'',t,l) \in FL} y_{f,f',f'',l,t} \cdot HC_{f,f',f'',t} = Cost_l^H \quad \forall l \in L \tag{21}$$

$$\sum_{(f,f',f'',t,l) \in FL} y_{f,f',f'',l,t} \cdot EC_{f,f',f'',t} = Cost_l^E \quad \forall l \in L \tag{22}$$

Note that the candidate facility hydrogen ($HC_{f,f',f'',t}$) and electricity ($EC_{f,f',f'',t}$) costs are readily determined if a fixed price of hydrogen and electricity is assumed (Eqs. (23) and (24), respectively):

$$HC_{f,f',f'',t} = HR_{f,f',f'',t} \cdot Cost_{H_2} \tag{23}$$

$$EC_{f,f',f'',t} = ER_{f,f',f'',t} \cdot Cost_{El} \tag{24}$$

If the hydrogen and electricity must come from a specific source (i.e., stream reforming of methane, coal gasification, or biomass gasification), then Eqs. (21) and (22) will not be sufficient because the different hydrogen/electricity generation technologies will have varying prices that depend on the type of technology and the layout of the energy supply chain network (Section 6.4).

The carbon-based feedstock requirement for each facility location ($FR_{f,l}$) is specified from the requirements for coal ($FR^{C}_{f,f',f'',t}$), biomass ($FR^{B}_{f,f',f'',t}$), and natural gas ($FR^{G}_{f,f',f'',t}$) for each candidate facility in Eqs. (25), (26) and (27), respectively:

$$FR_{f,l} = \sum_{(f,f',f'',t,l)\in FL} FR^{C}_{f,f',f'',t} \cdot y_{f,f',f'',l,t} \quad \forall f \in F^{C},\ l \in L \tag{25}$$

$$FR_{f',l} = \sum_{(f,f',f'',t,l)\in FL} FR^{B}_{f,f',f'',t} \cdot y_{f,f',f'',l,t} \quad \forall f' \in F^{B},\ l \in L \tag{26}$$

$$FR_{f'',l} = \sum_{(f,f',f'',t,l)\in FL} FR^{G}_{f,f',f'',t} \cdot y_{f,f',f'',l,t} \quad \forall f'' \in F^{G},\ l \in L \tag{27}$$

The feedstock requirements for the candidate facilities in Eqs. (25)–(27) are based on the requirement solely for the CBGTL process. If hydrogen and electricity are produced using one of these feedstocks, then the feedstock requirements must be augmented appropriately.

### 6.3.2. *Feedstock and product flow constraints*

The following equations constrain the coal, biomass, and natural gas feedstock flows from their source locations to the facility location. Given a feedstock source county (*f*, *c*), the total feedstock flow exiting the source via any mode of transportation *m* to the set of all accessible CBGTL facilities *FT* must not be greater than the available production from that particular source location (Eq. (28)). Additionally, given a facility feedstock requirement $FR_{f,l}$, the total flow of feedstock into the facility must be equal to the requirement (29):

$$\sum_{(f,c,l,m)\in FT} x_{f,c,l,m} \le FA_{f,c} \quad \forall (f,c) \in C_{F} \tag{28}$$

$$\sum_{(f,c,l,m)\in FT} x_{f,c,l,m} = FR_{f,l} \quad \forall f \in F,\ l \in L \tag{29}$$

Additional constraints must be added that limit the transportation of natural gas via interstate pipelines within the available capacities. Given the current capacity ($Cap_{m}$) and current usage ($Usage_{m}$) of each pipeline, the the available capacity for the CBGTL plant is specified using Eq. (30):

$$\sum_{(f,c,l,m)\in FT} x_{f,c,l,m} \le Cap_{m} - Usage_{m} \quad \forall m \in M^{G}_{Pipe},\ f \in F^{G} \tag{30}$$

The flow of gasoline, diesel, and kerosene products exiting every facility will be dictated by the production capacity ($Prod_{t}$) of each facility and the product ratios ($Ratio_{p}$) which are set in accordance with the United States demand ratio for the fuels (Eq. (31)). The total products produced in the energy supply chain must satisfy the demand amount for all appropriate counties in the United States (Eq. (32)):

$$\sum_{(p,l,c,m)\in PT} z_{p,l,c,m} = \sum_{(f,f',f'',t,l)\in FL} y_{f,f',f'',l,t} \cdot Prod_{t} \cdot Ratio_{p} \quad \forall l \in L,\ p \in P \tag{31}$$

$$\sum_{(p,c,l,m)\in PT} z_{p,l,c,m} = DM_{p,c} \quad \forall (p,c) \in C_{P} \tag{32}$$

### 6.4. *Alterations for specific hydrogen/electricity production*

Given a specific set of hydrogen production methods, *H*, each of the binary variables created from the set *FL* must be re-indexed to include the set of possible hydrogen and electricity production methods. Most constraints in the model will remain unaltered with the simple replacement of the binary variables from $y_{f,f',f'',t,l}$ to $y_{f,f',f'',t,l,h}$ and the set *FL* to $FL_{H}$:

$$FL_{H} = \{(f, f', f'', t, l, h) \in FL \times H\}$$

To address the appropriate changes in the model, the levelized cost for hydrogen and electricity production must be determined for each facility and each production method. The energy requirement for hydrogen and electricity is calculated using the lower heating value of hydrogen and the levelized cost for a hydrogen/electricity facility is calculated by assuming that only one feedstock will be input to the hydrogen production facility. This includes autothermal reforming for natural gas and gasification for biomass or coal. The feedstock types that are considered for hydrogen/electricity production are the same as those input to the CBGTL plant. The hydrogen and electricity costs are calculated by partitioning the levelized production cost ($LC^{H}_{f,f',f'',t,l,h}$) based on the energy needed for hydrogen or electricity:

$$HC_{f,f',f'',t,h} = LC^{H}_{f,f',f'',t,h} \cdot \frac{HR_{f,f',f'',t}}{HR_{f,f',f'',t} + ER_{f,f',f'',t}} \tag{33}$$

$$EC_{f,f',f'',t,h} = LC^{H}_{f,f',f'',t,h} \cdot \frac{ER_{f,f',f'',t}}{HR_{f,f',f'',t} + ER_{f,f',f'',t}} \tag{34}$$

Finally, the feedstock requirement of each facilility location must be altered to include both the input for the CBGTL process and the hydrogen/electricity production plant. Note that for a given feedstock type, the input to the hydrogen/electricity production plant ($FR^{H_2El}_{f,f',f'',t,h}$) will be equal to zero if that feedstock does not power the plant:

$$FR_{f,l} = \sum_{(f,f',f'',t,h)\in FL_{H}} (FR^{C-H_2El}_{f,f',f'',t,h} + FR^{C}_{f,f',f'',t}) \cdot y_{f,f',f'',l,t,h} \quad \forall f \in F^{C},\ l \in L \tag{35}$$

$$FR_{f',l} = \sum_{(f,f',f'',t,h)\in FL_{H}} (FR^{B-H_2El}_{f,f',f'',t,h} + FR^{B}_{f,f',f'',t}) \cdot y_{f,f',f'',l,t,h} \quad \forall f' \in F^{B},\ l \in L \tag{36}$$

$$FR_{f'',l} = \sum_{(f,f',f'',t,h)\in FL_{H}} (FR^{G-H_2El}_{f,f',f'',t,h} + FR^{G}_{f,f',f'',t}) \cdot y_{f,f',f'',l,t,h} \quad \forall f'' \in F^{G},\ l \in L \tag{37}$$

### 6.5. *Objective function*

The objective function includes the total overall cost of the energy supply chain network. Its components are (i) investment costs associated with the new CBGTL plants, (ii) feedstock purchase costs, (iii) feedstock and product transportation costs, and (iv) investment costs associated with necessary expansions of current transportation infrastructure:

$$\sum_{l\in L}(Cost^{I}_{l} + Cost^{H}_{l} + Cost^{E}_{l}) + \sum_{(f,c,l,m)\in FT} x_{f,c,l,m} \cdot (Cost^{F}_{f,c} + Cost^{FT}_{f,c,l,m}) + \sum_{(p,c,l,m)\in PT} z_{p,l,c,m} \cdot Cost^{PT}_{p,l,c,m} \tag{38}$$

Eqs. (16)–(32) and (38) represent a mixed-integer linear optimization (MILP) model that can be solved using CPLEX (2008) for the case of fixed hydrogen prices (i.e., case study 1). The model consists of 12,552 binary variables, 1,363,492 continuous variables, and 52,675 constraints. For case study 2 where distinct hydrogen production technologies are considered, the changes in parameter values need to be made as described in the previous section. Eqs. (33)–(34) would replace Eqs. (23)–(24), respectively, and Eqs. (35)–(37) would replace Eqs. (25)–(27), respectively. Eqs. (16)–(22) and (28)–(38) represent a MILP model for case study 2, which consists of 47,788 binary variables, 4,596,402 continuous variables, and 54,491 constraints. The models are solved using CPLEX to obtain (i) the active binary variables that represent the existence of a CBGTL plant and (ii) the amount of feedstock and product flows in the network. The overall topology of the network will show (a) the locations from which the three feedstocks are transported, (b) the interconnectivity between the feedstock sources, CBGTL plant locations, and the demand locations, and (c) the modes used for each transportation segment.

We note that the trade-offs between feedstock delivery cost, product delivery cost, and levelized investment cost are very slight for many locations throughout the country. This ultimately yields an MILP with a significant amount of degeneracy that makes it very difficult for CPLEX to find the optimal solution from the branch-and-bound tree. All computational studies performed in this paper have thus had an upper bound of 48 CPU hours for solution time and the incumbent solution with the smallest optimality gap is reported. The optimality gap was between 1 and 3% for all computational studies.

## 7. Computational studies

We investigate several factors that affect the layout of the optimal CBGTL network topology by conducting two case studies for alternative scenarios of carbon-based hydrogen production. Per unit mass, hydrogen is the most expensive feedstock required for the CBGTL process, so it is imperative to examine the effect of distinct hydrogen prices on the topology of the energy supply chain network. While future production of hydrogen may involve non-carbon-based systems such as nuclear, solar, and wind, coupled with electrolysis, further technological developments need to take place to make the capital cost of electrolyzer less dominant. Hydrogen at a lower cost, however, can be provided to the CBGTL process from coal, biomass, and natural gas via coal gasification, biomass gasification, and steam reforming of methane, respectively, with steam reforming of methane as the most prevailing technology today.

In case study 1, we present the CBGTL supply chain network with hydrogen supplied at four distinct prices (i.e., \$1.00, \$1.50, \$2.00, and \$2.50/kg $H_2$), assuming that hydrogen is produced via steam reforming of methane. Feedstock locations and availabilities are considered only for the CBGTL process and not for the hydrogen production. In case study 2, the changes in the CBGTL supply chain network are analyzed when selections on the carbon-based hydrogen production technologies are taken into account. Hydrogen may be produced via a coal, biomass, or natural gas system, and the optimization model selects the best and most economical technology for each of the selected CBGTL plant. Additionally, the feedstock locations and availabilities for both the CBGTL process and the hydrogen production are taken into account.

For each case study, the environmental performance of the CBGTL network is assessed via a life cycle analysis to obtain an overall GHG emissions for the country. In the discussions on the network topology, state groupings are based on the regional definitions based on the 10 Federal Regions of the U.S. Bureau of Labor Statistics from the EIA website (Energy Information Administration, 2010b), which can be found in Table 8.

**Table 8**
State groupings and regional definitions of the United States. The grouping defined here is based on the 10 Federal Regions of the U.S. Bureau of Labor Statistics, as published on the EIA website (Energy Information Administration, 2010b).

| Region | States |
|---|---|
| Northeast | CT, ME, MA, NH, RI, VT, NJ, NY, DE, DC, MD, PA, VA, WV |
| Southeast | AL, FL, GA, KY, MS, NC, SC, TN |
| Midwest | IL, IN, MI, MN, OH, WI |
| Southwest | AR, LA, NM, OK, TX |
| Central | IA, KS, MO, NE, CO, MT, ND, SD, UT, WY |
| Western | AZ, CA, NV, ID, OR, WA |

### 7.1. *Case study 1: carbon-based hydrogen at distinct prices*

In case study 1, we assume that hydrogen is available at a fixed price for the entire energy supply chain network. We assume that hydrogen is produced via steam reforming of methane, which is currently the main route of hydrogen production. For this analysis, we have chosen to investigate the hydrogen costs of \$1.00/kg, \$1.50/kg, \$2.00/kg, and \$2.50/kg to represent the cost range for current and future cases of centralized hydrogen plants with and without sequestration (National Research Council, 2004).

The cost of fuels and the number of plants selected in the energy supply chain network for all four runs are presented in Table 9. The overall cost represents the total levelized cost to supply transportation fuels for the entire country divided by the total lower heating value (LHV) of those transportation fuels. The breakeven crude oil price (BEOP) for the CBGTL supply chain network is defined as the price of crude oil in \$ per barrel at which the resale prices of liquid fuel products from petroleum based processes are equal to the cost of producing fuels in the CBGTL supply chain network (Kreutz, Larson, Liu, & Williams, 2008; Larson et al., 2010). This value is obtained by subtracting the refinery margin (RM), which is the difference between the refinery sale price of petroleum products and the purchase price of crude oil, from the overall cost in \$/GJ LHV (Baliban et al., 2010; Kreutz et al., 2008). The RM is taken to be \$0.333/gal, \$0.266/gal, and \$0.217/gal for gasoline, diesel, and kerosene, respectively, based on the average over the period of 1992–2003, adjusted with the U.S. Gross Domestic Index (Baliban et al., 2010). The RM for diesel is \$0.05/gal higher than the average due to the additional cost for the production of low-sulfur diesel (Kreutz et al., 2008).

Based on this calculation, the overall cost of producing transportation fuels in the CBGTL supply chain network is equal to \$15.68/GJ LHV of fuel produced if hydrogen is available at \$1.00/kg, which is equivalent to \$76.55/bbl of crude oil. Compared to the United States crude oil prices in 2010, which range from \$65.45 to \$81.64/bbl (Energy Information Administration, 2010c), the CBGTL supply chain network is economically competitive with petroleum based fuels at \$1.00/kg hydrogen. The overall costs of subsequent case study 1 runs are \$17.67/GJ (\$87.89/bbl) for \$1.50/kg hydrogen, \$19.84/GJ (\$100.26/bbl) for \$2.00/kg hydrogen, and \$22.06/GJ (\$112.91) for \$2.50/kg hydrogen. The fuel products are produced in mostly medium-sized facilities, as shown in Table 9. This is likely a result of the trade-off between carbon-based feedstock availabilities and the process' economies of scale. Larger facilities gain more economies of scale, but would require more coal, biomass, and natural gas feedstocks from their surrounding areas, which may or may

**Table 9**
Overall results of case study 1.

| Hydrogen cost (\$/kg) | Product cost (\$/GJ$_{LHV}$) | BEOP [a] (\$/bbl) | Total number of facilities | | |
|---|---|---|---|---|---|
| | | | Small | Medium | Large |
| \$1.00 | \$15.68 | \$76.55 | 39 | 124 | 33 |
| \$1.50 | \$17.67 | \$87.89 | 44 | 127 | 32 |
| \$2.00 | \$19.84 | \$100.26 | 44 | 123 | 33 |
| \$2.50 | \$22.06 | \$112.91 | 44 | 123 | 33 |

[a] BEOP – breakeven oil price.

**Table 10**

Topology of the entire supply chain network for case study 1 with $1.00/kg $H_2$, discretized by regions. The leftmost column displays the region where the facilities are located. The horizontal tab for the first and second part of the table represents the regions of feedstock origins and the regions of product destination, respectively (e.g., facilities in the northeast region of the United States receive 96.69% incoming coal from within the northeast region and 3.31% from the midwest region. They subsequently deliver 88.48% of produced gasoline within the region and 11.52% to the southeast region.

| Facility region | Feedstock type | Region of feedstock origin | | | | | |
|---|---|---|---|---|---|---|---|
| | | Northeast | Southeast | Midwest | Southwest | Central | Western |
| Northeast | Coal | 96.69% | – | 3.31% | – | – | – |
| | Biomass | 45.39% | 24.52% | 25.36% | 1.01% | 1.89% | 1.81% |
| | Natural gas | 100.00% | – | – | – | – | – |
| Southeast | Coal | 46.52% | 33.39% | 7.22% | 12.88% | – | – |
| | Biomass | 1.68% | 57.19% | 13.41% | 8.75% | 3.68% | 15.28% |
| | Natural gas | 15.10% | 32.93% | – | 51.97% | – | – |
| Midwest | Coal | 22.37% | – | 77.63% | – | – | – |
| | Biomass | 7.13% | 0.94% | 89.82% | 0.29% | 1.82% | – |
| | Natural gas | 13.91% | – | 51.80% | 34.29% | – | – |
| Southwest | Coal | 5.36% | 3.12% | 8.42% | 81.37% | 1.74% | – |
| | Biomass | 2.32% | 27.69% | 5.00% | 44.69% | 6.96% | 13.34% |
| | Natural gas | – | – | – | 100.00% | – | – |
| Central | Coal | – | – | 36.13% | 3.26% | 60.60% | – |
| | Biomass | 1.09% | 0.02% | 7.73% | 2.89% | 86.54% | 1.72% |
| | Natural gas | – | – | – | 36.95% | 63.05% | – |
| Western | Coal | – | – | – | 7.64% | 40.37% | 51.99% |
| | Biomass | 3.04% | – | 5.69% | 22.41% | 11.10% | 57.76% |
| | Natural gas | – | – | – | 7.02% | 34.11% | 58.87% |

| Facility region | Product type | Region of product destination | | | | | | HI | AK |
|---|---|---|---|---|---|---|---|---|---|
| | | Northeast | Southeast | Midwest | Southwest | Central | Western | | |
| Northeast | Gasoline | 88.48% | 11.52% | – | – | – | – | – | – |
| | Diesel | 88.37% | 8.72% | 2.91% | – | – | – | – | – |
| | Kerosene | 70.55% | 11.63% | 0.38% | – | – | 17.44% | – | – |
| Southeast | Gasoline | 17.14% | 57.71% | 15.15% | – | – | 10.00% | – | – |
| | Diesel | 11.74% | 54.10% | 16.14% | 7.08% | 5.23% | 5.70% | – | – |
| | Kerosene | 21.46% | 34.26% | 10.11% | 6.52% | – | 27.65% | – | – |
| Midwest | Gasoline | 20.00% | 11.91% | 67.39% | – | 0.70% | – | – | – |
| | Diesel | 8.57% | 16.89% | 72.38% | – | 2.16% | – | – | – |
| | Kerosene | 8.57% | 13.49% | 46.86% | – | 7.05% | 14.92% | 9.11% | – |
| Southwest | Gasoline | 12.82% | 9.42% | – | 27.04% | 5.74% | 44.98% | – | – |
| | Diesel | – | – | – | 47.11% | 15.53% | 37.36% | – | – |
| | Kerosene | 16.34% | 5.88% | 0.59% | 42.37% | 1.68% | 31.11% | 2.03% | – |
| Central | Gasoline | 2.30% | 0.17% | 11.97% | 37.87% | 28.02% | 17.68% | 1.23% | 0.77% |
| | Diesel | – | – | 10.58% | 41.70% | 28.87% | 16.66% | 1.05% | 1.14% |
| | Kerosene | 2.90% | – | 13.06% | 42.47% | 14.70% | 24.95% | 1.93% | – |
| Western | Gasoline | – | – | – | – | 6.86% | 93.14% | – | – |
| | Diesel | – | – | – | – | 3.36% | 87.87% | – | 8.77% |
| | Kerosene | 1.75% | – | 1.30% | – | 17.54% | 69.23% | – | 10.17% |

not be able to supply the required amounts. If the surrounding areas cannot supply the required amounts of feedstocks, the facilities would need to draw resources from farther locations, increasing the costs of transportation. To further investigate the network topology, a more detailed discussion on the results of the first run (i.e., hydrogen at a fixed price of $1.00/kg) is presented in the following subsections.

### 7.1.1. *Individual facility costs*

For a fixed hydrogen price of $1.00/kg, a total of 196 facilities were selected in the optimal energy supply chain network, including 39 small (10,000 BPD), 124 medium (50,000 BPD), and 33 large (200,000 BPD) facilities. Though the country is able to provide liquid fuels at an average price of $15.68/GJ ($76.55/bbl), it is important to analyze the selling price for each individual facility. Firstly, this can provide perspective on the relative costs for each plant and the trade-offs between feedstock types and plant sizes. Second, it will be possible to identify the plant locations that can provide fuels at the lowest cost, thereby providing targets for initial CBGTL facility development. For illustration purposes, Fig. 7 presents the breakdown of the costs for 7 facilities in the state of Missouri, which is one of the states with the highest number of large plants in the energy supply chain network. For the complete set of results that includes each selected facility in the energy supply chain network, please consult the Supporting Information provided along with this paper. The most significant contributing factors in the cost distribution are the cost of hydrogen purchase and biomass transportation by truck. Note that the horizontal labels are of the form S*s* O*o* where *s* represents the FIPS designation for the state and *o* represents the octant where the facility is located. Octant *o* = 1 corresponds to the NNE (North-Northeast) section, and the remaining octants are indexed by traversing clockwise around the state. That is, octant *o* = 2 corresponds to the ENE (East-Northeast) section and so forth.

The average cost for the small plants in the network is $17.97/GJ ($89.60/bbl), while the average cost for medium and large plants are $16.22/GJ ($79.63/bbl) and $15.04/GJ ($72.90/bbl), respectively. The decrease in cost as the plant size increases is due to the economies of scale of the plant capital costs. Note that even though

**Table 11**
Topology of the entire supply chain network for case study 2. The leftmost column displays the region where the facilities are located. The horizontal tab for the first and second part of the table represents the regions of feedstock origins and the regions of product destination, respectively (e.g., facilities in the northeast region of the United States receive 98.26% incoming coal from within the northeast region and 1.74% from the midwest region. They subsequently deliver 79.09% of produced gasoline within the region and 20.91% to the southeast region.

| Facility region | Feedstock type | Region of feedstock origin | | | | | |
|---|---|---|---|---|---|---|---|
| | | Northeast | Southeast | Midwest | Southwest | Central | Western |
| Northeast | Coal | 98.26% | – | 1.74% | – | – | – |
| | Biomass | 49.15% | 14.61% | 27.51% | 1.41% | 4.29% | 3.02% |
| | Natural gas | 100.00% | – | – | – | – | – |
| Southeast | Coal | 34.98% | 28.11% | 31.12% | 5.79% | – | – |
| | Biomass | 1.89% | 46.54% | 23.78% | 13.20% | 14.43% | 0.16% |
| | Natural gas | 7.97% | 21.88% | – | 70.15% | – | – |
| Midwest | Coal | 2.32% | – | 97.68% | – | – | – |
| | Biomass | 7.67% | 2.20% | 75.91% | 0.10% | 13.78% | 0.34% |
| | Natural gas | 15.56% | 10.19% | 42.96% | 30.81% | 0.47% | – |
| Southwest | Coal | 3.35% | – | 3.02% | 91.78% | 0 | 1.84% |
| | Biomass | 2.75% | 21.98% | 4.15% | 30.90% | 37.91% | 2.33% |
| | Natural gas | – | – | – | 99.93% | 0.07% | – |
| Central | Coal | – | 0.04% | 1.50% | 5.64% | 92.73% | 0.09% |
| | Biomass | 0.67% | – | 9.61% | 2.53% | 86.78% | 0.41% |
| | Natural gas | – | – | – | 7.22% | 92.78% | – |
| Western | Coal | – | – | – | 13.06% | 73.26% | 13.69% |
| | Biomass | 0.16% | – | 0.43% | 2.16% | 14.88% | 82.36% |
| | Natural gas | – | – | – | 6.19% | 73.49% | 20.32% |

| Facility region | Product type | Region of product destination | | | | | | HI | AK |
|---|---|---|---|---|---|---|---|---|---|
| | | Northeast | Southeast | Midwest | Southwest | Central | Western | | |
| Northeast | Gasoline | 79.09% | 20.91% | – | – | – | – | – | – |
| | Diesel | 83.05% | 16.95% | – | – | – | – | – | – |
| | Kerosene | 86.08% | 9.30% | – | 4.61% | – | 0.01% | – | – |
| Southeast | Gasoline | 9.65% | 75.29% | 8.03% | – | – | 4.69% | 1.44% | 0.90% |
| | Diesel | 9.03% | 68.08% | 10.47% | 3.94% | – | 7.61% | – | 0.87% |
| | Kerosene | 17.63% | 34.16% | 2.35% | 1.69% | – | 43.27% | – | 0.89% |
| Midwest | Gasoline | 26.91% | 9.88% | 63.21% | – | – | – | – | – |
| | Diesel | 21.90% | 11.85% | 63.33% | – | 2.92% | – | – | – |
| | Kerosene | 16.59% | 16.99% | 57.50% | 3.24% | – | – | 5.68% | – |
| Southwest | Gasoline | 27.65% | 6.42% | – | 28.57% | – | 37.36% | – | – |
| | Diesel | 3.05% | 4.47% | 1.66% | 56.42% | 1.20% | 33.20% | – | – |
| | Kerosene | 17.35% | – | – | 43.65% | – | 38.70% | – | 0.30% |
| Central | Gasoline | 6.13% | 0.06% | 15.69% | 31.66% | 27.89% | 18.58% | – | – |
| | Diesel | 0.52% | – | 16.33% | 35.48% | 36.09% | 11.59% | – | – |
| | Kerosene | 1.25% | 9.76% | 10.41% | 37.25% | 18.97% | 18.18% | 3.52% | 0.66% |
| Western | Gasoline | – | – | – | – | – | 100.00% | – | – |
| | Diesel | – | – | – | – | – | 87.01% | 4.07% | 8.29% |
| | Kerosene | – | – | – | – | – | 100.00% | – | – |

the number of large plants in this network is only 33, the total fuel produced by large plants is actually larger than that produced by the 124 medium plants in the network (i.e., a total of 6,600,000 BPD produced by large plants as opposed to 6,200,000 BPD produced by medium plants). Hence, the amount of fuel produced is inversely correlated with the cost of production and centralized production of fuels in large plants is more profitable. However, the small plants are still necessary to meet the exact demands of the country as well as to accommodate locations with scarcer resources.

There are 66 facilities where the total cost to produce products is $15/GJ or less. KY, MD, OH, PA, TN, VA, and WV each provides at least four low cost facilities at different octants in the state. Facilities with the highest overall costs are located in AL, AZ, CA, GA, NV, and UT, with the two highest costs being located in CA ($25.77/GJ; $134.05/bbl) and NV ($24.52/GJ; $126.93/bbl). These locations tend to be in the western part of the country where coal and biomass are scarce, and in the southeastern part of the country. The cost distribution of these plants are consistently dominated by the cost of delivered biomass to the facility.

### 7.1.2. Network layout

To further understand the individual facility product costs, the facility locations in the energy supply chain network are presented in Fig. 8. The CBGTL facilities are represented as green circles and the states have been colored to show the relative quantities of coal, biomass, and natural gas feedstocks. We first note the string of large facilities that exist in the midwest region of the county, where the supplies of biomass feedstock are the most prevalent. However, in the southern and northeastern sections of the county, the selection of medium plants is preferred. The southeastern states have a mixture of medium and large facilities, and the small facilities are common in the southwest and northwestern states.

Figs. 9–11 focus on the flows of feedstock to the large facilities in NE, KS, and MO (i.e., the three states that have the highest number of large facilities). For each facility, the coal, biomass, and natural gas feedstocks may come from multiple sources in various states. This is especially true for biomass whose production is more widespread than coal and natural gas. From Fig. 9, we observe that WY supplies all the coal for the facilities in NE and one of the large facilities in KS. Additionally, KS receives coal from CO, IL, and MO, while all the large facilities in MO receive coal from IL. Note that the arrows only represent the connections between coal sources and flow destinations, and do not represent the actual pathway of coal transportation by rail. Fig. 10 shows the states that supply biomass to each of the large facilities in the three states. Since IA does not have any facility selected in its region, it channels its abundant biomass resources to the neighboring states. Since the midwest area is generally abundant in biomass, the transportation

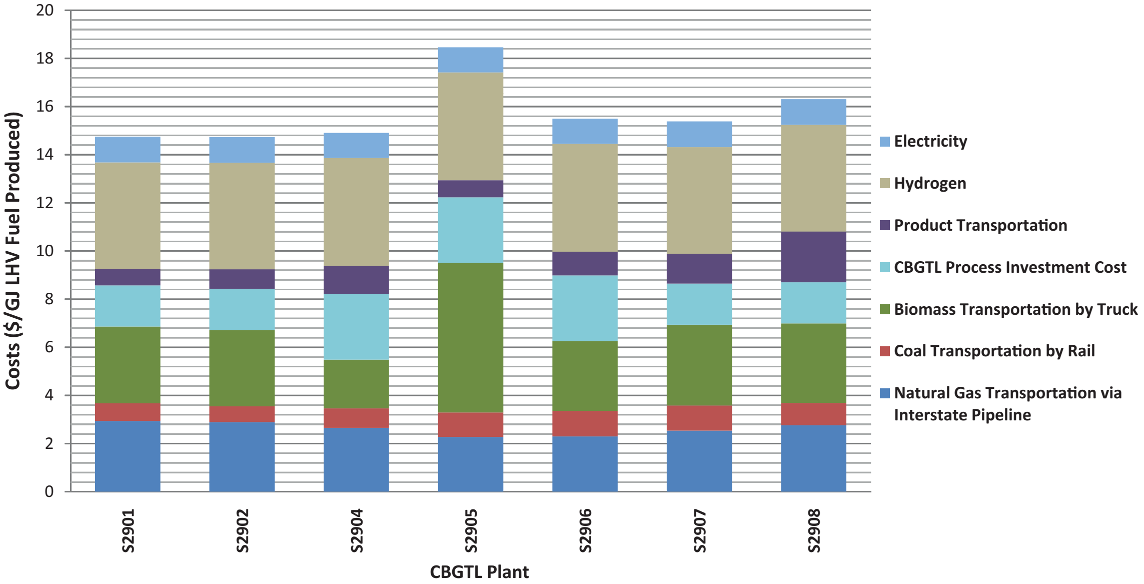

**Fig. 7.** Product costs for 7 facilities in the state of Missouri. All costs are reported in $/GJ of lower heating value (LHV) of the total products produced. Each facility is represented as S*s* O*o* where *s* represents the FIPS state designation (see the Supporting Information) and *o* represents the octant for the particular state. Octant *o* = 1 corresponds to the NNE section, and the remaining octants are increasingly indexed by traversing clockwise around the state. The coal, biomass, natural gas (NG), and hydrogen feedstock prices represent "as-received", delivered to the plant gate prices for the corresponding method of transportation. Electricity prices are based on a $0.07/kWh cost at the plant gate. The levelized investment cost of each facility is based on the fixed capital charges and operating/maintenence costs resulting from the total overnight capital of each plant. Note that natural gas and coal were not delivered by truck in the optimal CBGTL network configuration.

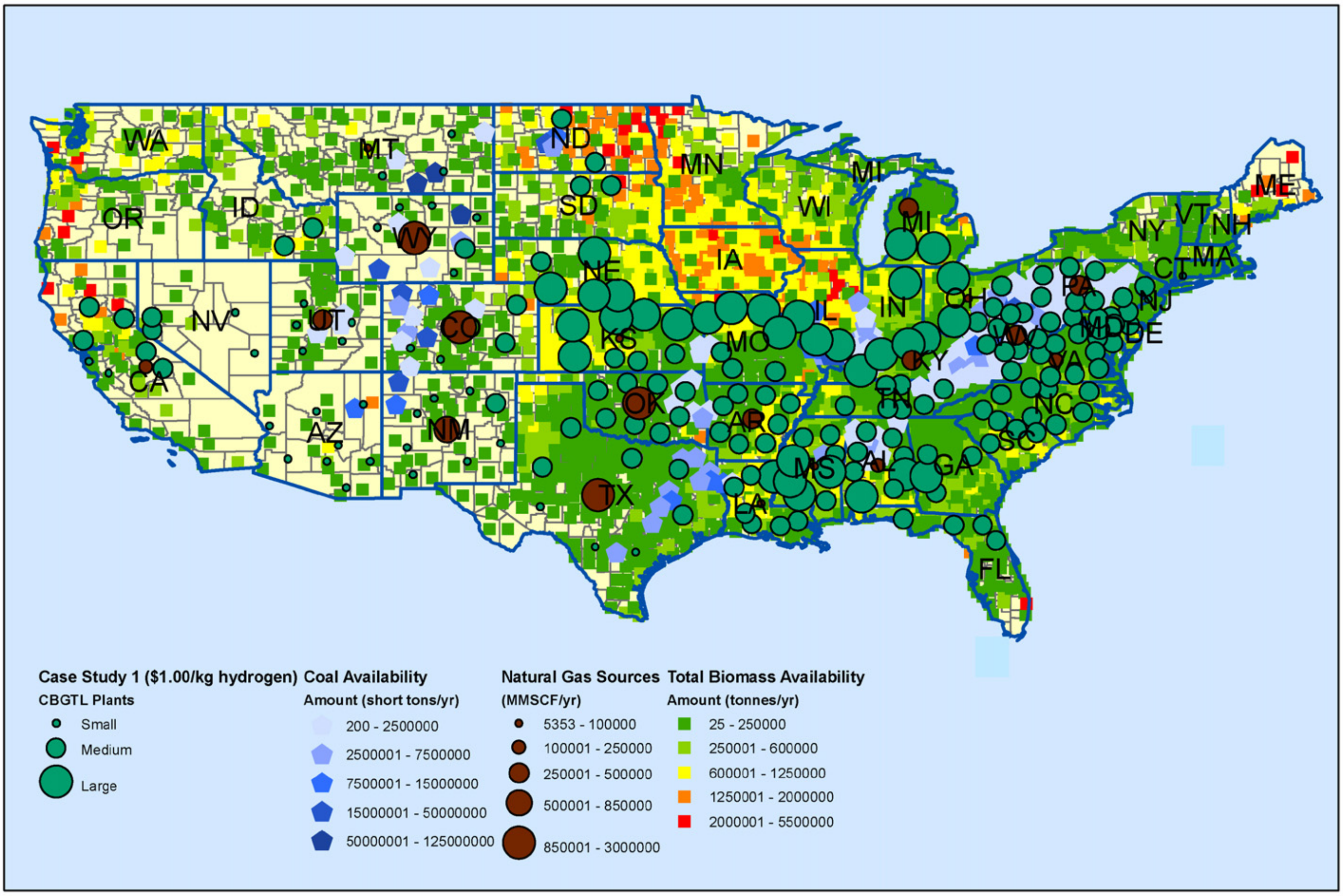

**Fig. 8.** Case study 1 selected facility locations at a fixed hydrogen price of $1.00/kg. Each facility is represented by a green circle centered at the proposed facility location, with the size of the circle signifying the size of the plant. The amounts of coal, biomass, and natural gas feedstock in the United States are also represented as the background of the map. The brown circles signify the sources of natural gas, the blue pentagons represent coal sources, and the green, yellow, and red squares signify biomass sources. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

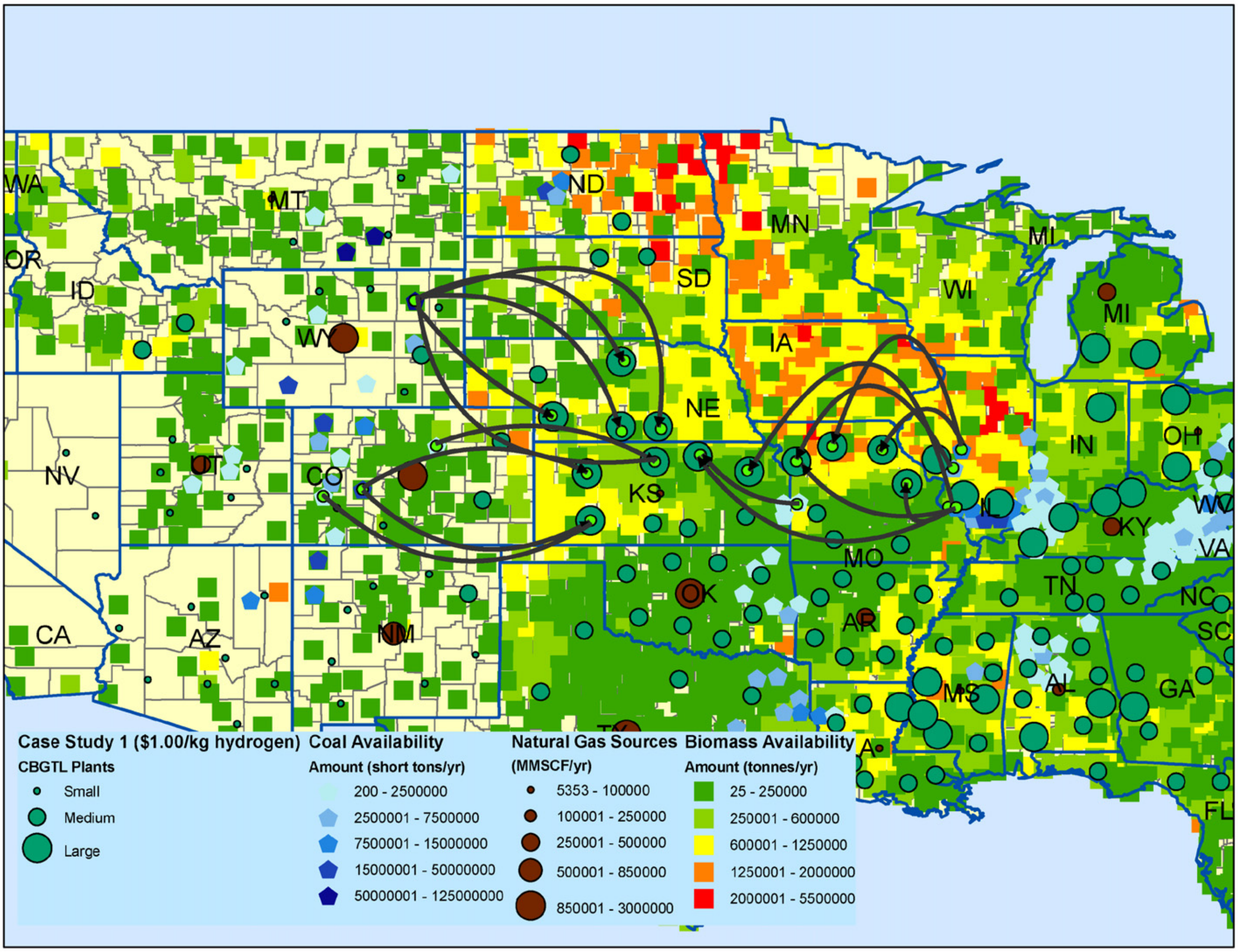

**Fig. 9.** The flow of coal feedstock to selected large facilities in NE, KS, and MO for case study 1. The arrows connect the origin of coal feedstock to the facility locations, and these connected points are represented by the small light green circles. Note that the edges do not represent the actual pathway of coal transportation by rail. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

distance can be kept at a low level, especially since the delivered cost of biomass tends to be high. Note that for each facility, biomass can come from many different counties from various states, but for simplicity, only the originating states are represented on the map. In other words, the white circles do not represent the actual feedstock location. Lastly, natural gas to these three states are mostly fulfilled by WY, CO, and OK, as shown in Fig. 11.

The states that do not have facilities in their region include AK, HI, IA, ME, MA, MN, NH, NY, OR, RI, VT, WA, and WI. Due to unavailable infrastructure to deliver coal, biomass, and natural gas feedstock to facilities in AK and HI, they are always excluded from the selection of CBGTL facility locations. Delivery of products to these two states, however, are allowed via barges from the lower 48 states and pipelines once they reach the designated states. The rest of the states that do not have any CBGTL facilities is consistent among the different runs in this case study. We observe that these "empty" states are located in the northern parts of the United States and all of them do not have coal and natural gas resources within their boundaries. Additionally, the natural gas pipeline infrastructures in these states are more sparse than the rest of the country (Energy Information Administration, 2009b), meaning that to place facilities in these states, extensive amount of pipeline expansions need to take place. The cost of this expansion may be significant and it would be more profitable for the network to produce fuel products elsewhere. Other states without either coal or natural gas resources (i.e., CT, DE, DC, FL, GA, ID, NE, NV, NJ, NC, SC, and SD) that are selected in the CBGTL network tend to be more south and in closer proximity to feedstock sources, thus are more accessible for the delivery of feedstock.

The movements of feedstock and products for facilities in the western region are mostly contained within the region. The region receives additional coal and natural gas from the central and southwest regions and delivers the majority of its products within the western region. Additionally, the western region also receives quite a large portion of gasoline, diesel, and kerosene from the southwest region (44.98%, 37.36%, and 31.11% of southwest production, respectively). The southwest region fulfills all of its natural gas requirement and most of its coal requirement, but it takes biomass from all six regions of the country. Kerosene demands in HI are mostly fulfilled by the midwest region, with the rest fulfilled by production in the southwest and central regions. For AK, all of its kerosene demands and most of its diesel demands are supplied from the western region, with a small amount supplied by the central region.

The midwest and northeast regions supply most of their feedstock requirements within the region. The midwest area is

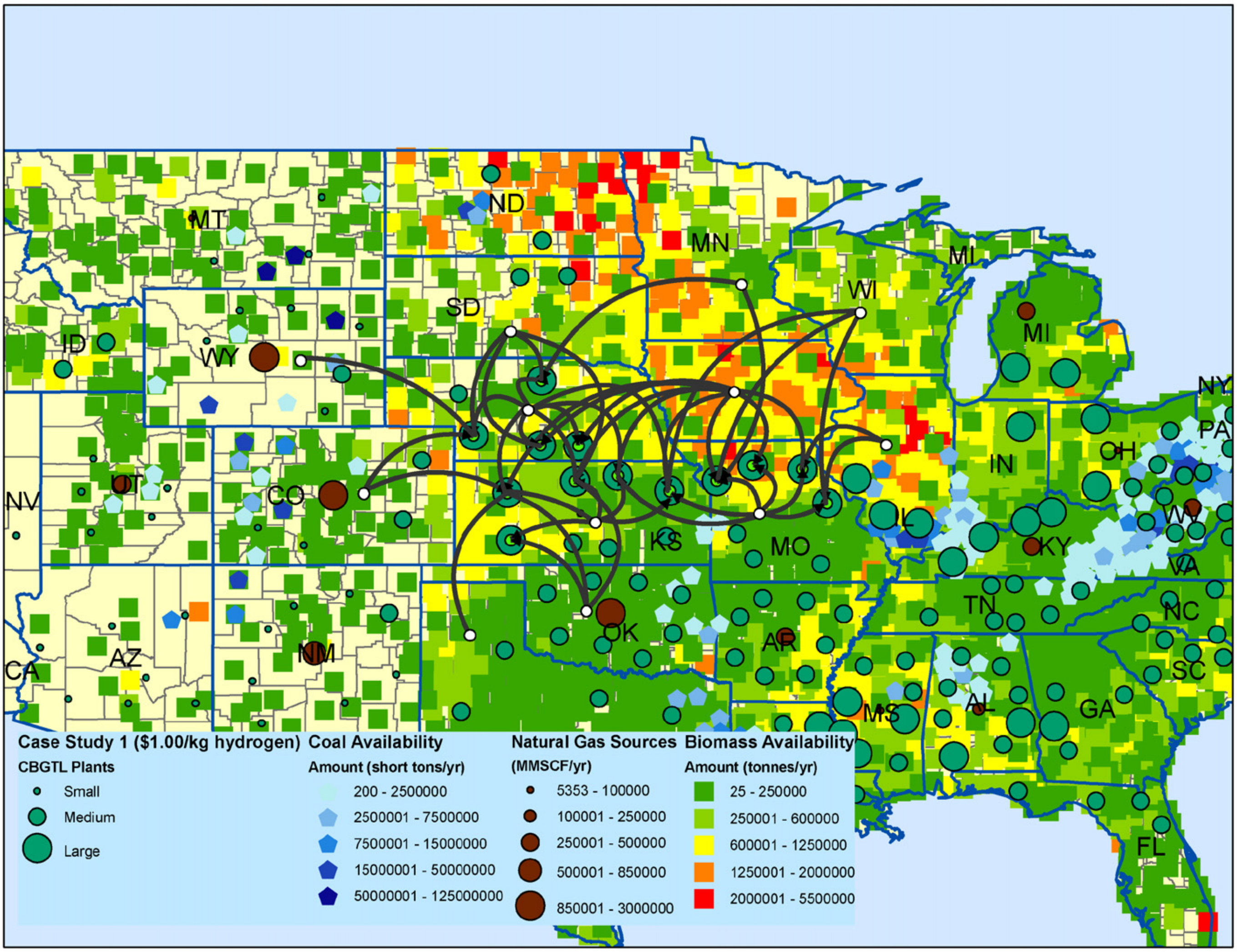

**Fig. 10.** The flow of biomass feedstock to selected large facilities in NE, KS, and MO for case study 1. The arrows connect the origin of biomass feedstock, which are represented by the white circles, to the facility locations, represented by the light green circles. Note that for each facility, biomass comes from many different counties from various states, but for simplicity, only the originating states are represented (i.e., the white circles do not represent the actual feedstock location). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

abundant in coal and biomass, and thus can fulfill 77.63% and 89.82% of its requirements, respectively, and can supply biomass to the other regions. The midwest natural gas input requires additional production from the northeast and southwest regions, both of which can supply 100% of their natural gas requirements. A representation of the topology of the southeast region is displayed in Fig. 12. The feedstock distribution charts represent the various regions that facilities in the southeast region draw their inputs from, and the product distribution charts represent the regions that receive products from the production in the southeast region. The overall amounts of feedstock and products delivery in the network, discretized by regions, are shown in Table 10.

### *7.1.3. Life cycle analysis*

The life cycle analysis is completed for each of the selected plants to estimate the true GHG emission for the energy supply chain network (see Appendix A). With the known amounts of feedstock and product flows, as well as the distances traveled by each commodity, the GHG emissions for each segment of the energy supply chain can be calculated. For the intermodal transport of liquid fuel products, each facility's contribution to the transportation emissions of each segment (i.e., transport via pipelines from facility to port, transport via barges from port to port, and transport via pipelines from port to demand locations) is calculated based on the amount of products that the facility sends to the ports.

The total greenhouse gas (GHG) emissions in $CO_2$ equivalents ($CO_{2eq}$) for the 7 selected facilities in the state of Missouri are presented in Fig. 13. For the complete life cycle analysis for each selected facility in the supply chain network, please see the Supporting Information. When selecting the carbon-based feedstock composition for a CBGTL process, the goal was to achieve a 50% reduction in GHG emissions for each plant from petroleum based processes. Note that the feedstock composition was selected based on assumed transportation distances for each plant, and therefore the GHG emissions from the case study will be different from those predicted earlier (see Appendix A). The average emissions for the network with $1.00/kg hydrogen is 43.40 kg $CO_{2eq}$/GJ LHV fuel produced, slightly lower than 50% of petroleum based processes, and the range of individual facility emissions is 14.14–53.50 kg $CO_{2eq}$/GJ LHV fuel produced.

In general, the largest contributing factor to the overall emissions comes from the consumption of the produced liquid fuels. Apart from fuel consumption, other significant factors include the hydrogen production, which is assumed to be produced via

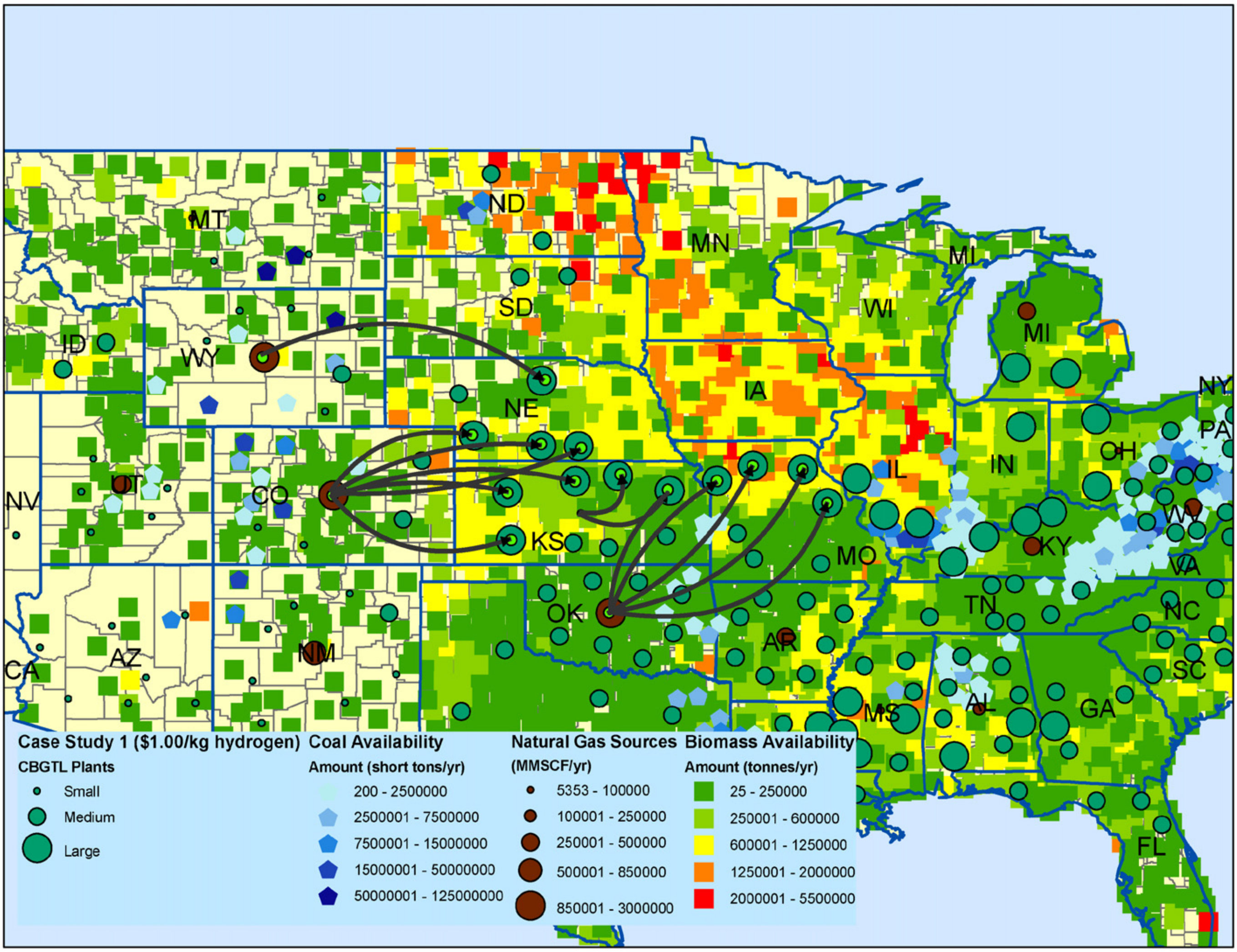

**Fig. 11.** The flow of natural gas feedstock to selected large facilities in NE, KS, and MO for case study 1. The arrows connect the origin of natural gas feedstock to the facility locations, and these connected points are represented by the small light green circles. Note that the edges do not represent the actual pathway of natural gas transportation by pipeline. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

steam reforming of methane, and the transportation of biomass to the facility location. The negative contribution comes from the carbon storage during biomass cultivation. The orange bar at 91.6 kg $CO_{2eq}$/GJ fuel represents the current GHG emissions for petroleum based processes. In some cases, the GHG emissions are significantly lower than the 50% target, corresponding to facilities that use switchgrass as biomass feedstock, which have additional benefit of soil sequestration of carbon during biomass cultivation. The mathematical model for the supply chain network did not assume any benefit for $CO_2$ avoided based on the use of a specific biomass feedstock, so only 10 facilities utilize switchgrass in the energy supply chain network. Facilities with higher $CO_2$ emissions have larger emissions contribution from biomass transportation, corresponding to the facilities with higher overall costs due to biomass transportation. Since biomass is transported by truck, both the high cost and emission figures can be attributed to the distance that biomass has to travel to the facilities.

### *7.1.4. Comparisons*

With the increase of hydrogen price, the layout of the energy supply chain network is generally consistent. Slight variations are observed in the increase of the number of small-sized plants to accommodate the reduction in the number of medium-sized plants, so that the total amount of demands for the country is still fulfilled. However, even though the number of plants is consistent, more variations exist in the types of selected CBGTL plants. These variations occur because the changes in hydrogen prices directly affect the selection of the facility type (i.e., a certain combination of coal, biomass, and natural gas feedstock and plant size), each of which has a distinct value of hydrogen requirement for the process. For example, a small facility in the first octant of AZ is always selected in the four runs of case study 1. At $1.00/kg hydrogen, high-volatile bituminous coal and softwood are selected as coal and biomass feedstock, respectively. The plant requires 3.66 kg/s of hydrogen input. In the subsequent runs of case study 1, the selected plant utilizes high-volatile bituminous coal and urban waste as feedstocks instead. This plant only requires 3.16 kg/s of hydrogen input. It should be noted that this shift of plant types among the different runs is also affected by the availabilities of the feedstock in the surrounding areas. The change of plant type at one location will be affected by the feedstock selections of nearby plants, and the shift to lower hydrogen input may not occur for all facilities. However, the overall supply chain network selects the CBGTL plants with a lower total of hydrogen requirements for the entire country.

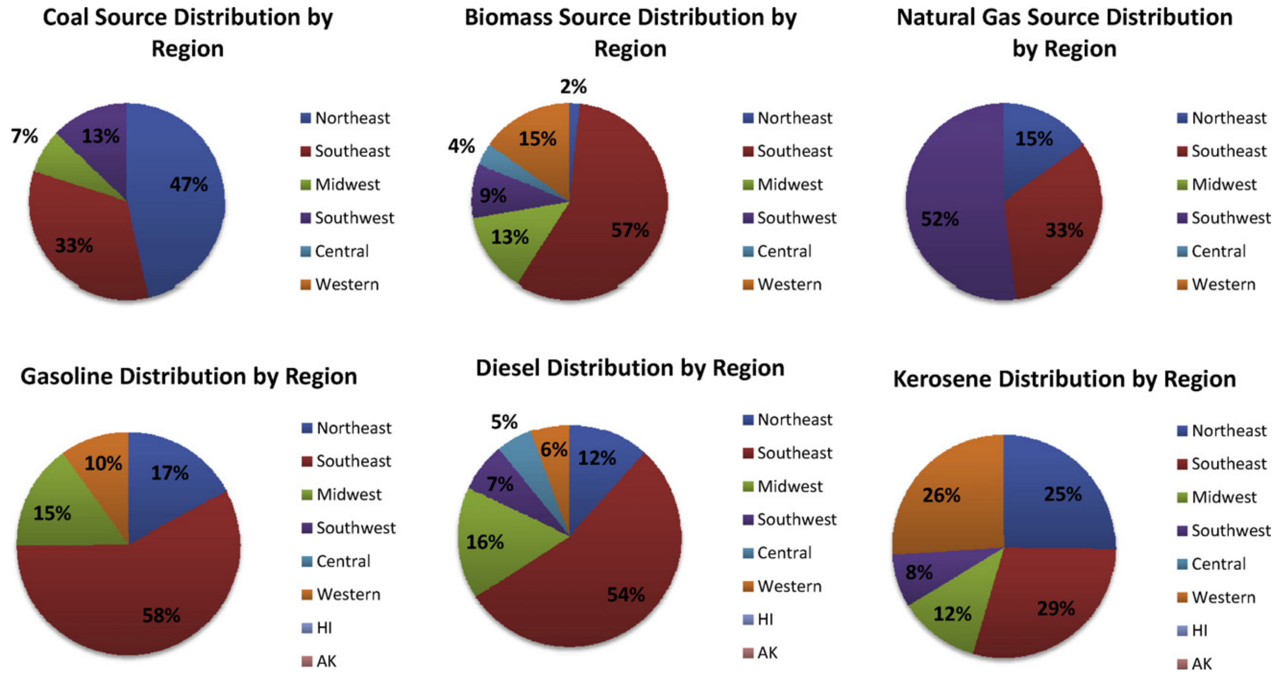

**Fig. 12.** The topology for the southeast region for case study 1 at a fixed hydrogen price of $1.00/kg. The feedstock distribution charts represent the various regions that facilities in the southeast region draw their inputs from, and the product distribution charts represent the regions that receive products from the production in the southeast region.

## *7.2. Case study 2: alternative technologies for carbon-based hydrogen production*

In case study 2, we consider hydrogen production from three carbon-based options, namely production from biomass, coal, or natural gas reforming. Due to the high amount of hydrogen needed by the CBGTL process, a single carbon source would not be able to fulfill the hydrogen demand of the network for the entire country and thus, a combination of hydrogen production from biomass, coal, and natural gas would be required. Each CBGTL facility is assumed to have one hydrogen production plant installed on-site, selecting one out of the three technology options. The biomass or

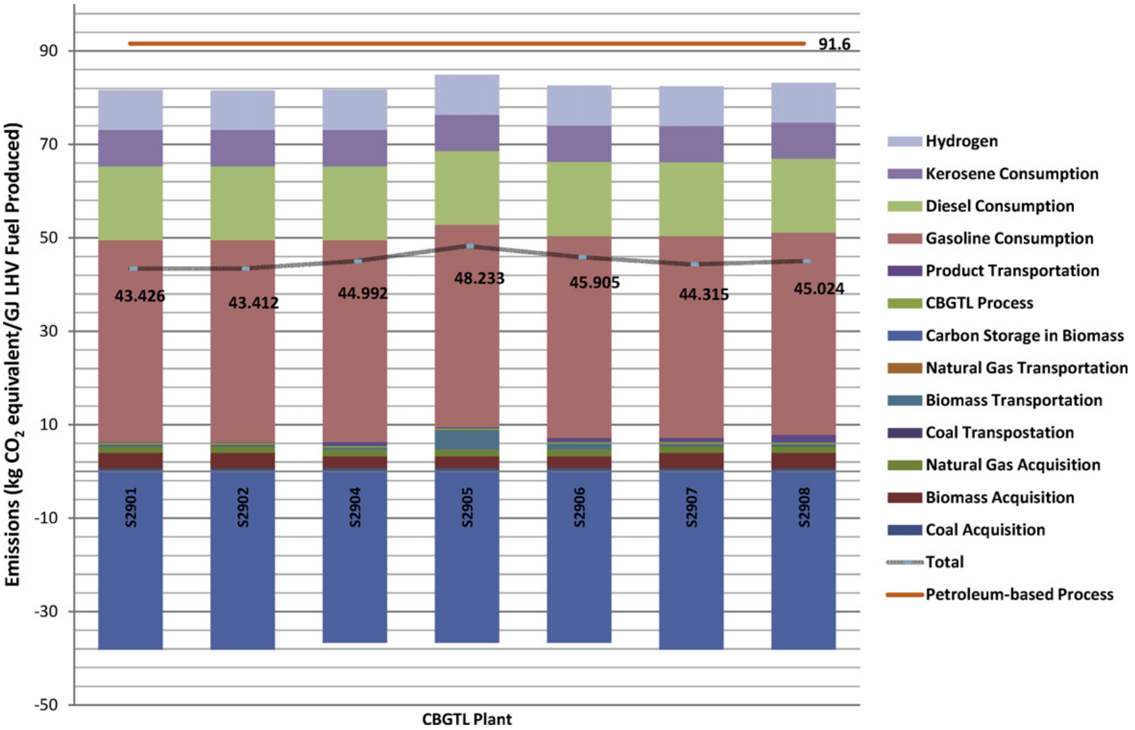

**Fig. 13.** Case study 1 greenhouse gas emissions at $1.00/kg hydrogen for 7 selected facilities in the state of Missouri. The current emissions for petroleum based processes is equal to 91.6 kg $CO_{2eq}$/GJ fuel and is represented by the orange bar. The total emissions for each facility is represented by the blue square along the connecting black line. On average, the total emissions per GJ LHV fuel produced in the supply chain network is slightly lower than 50% of the emissions from petroleum based processes. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

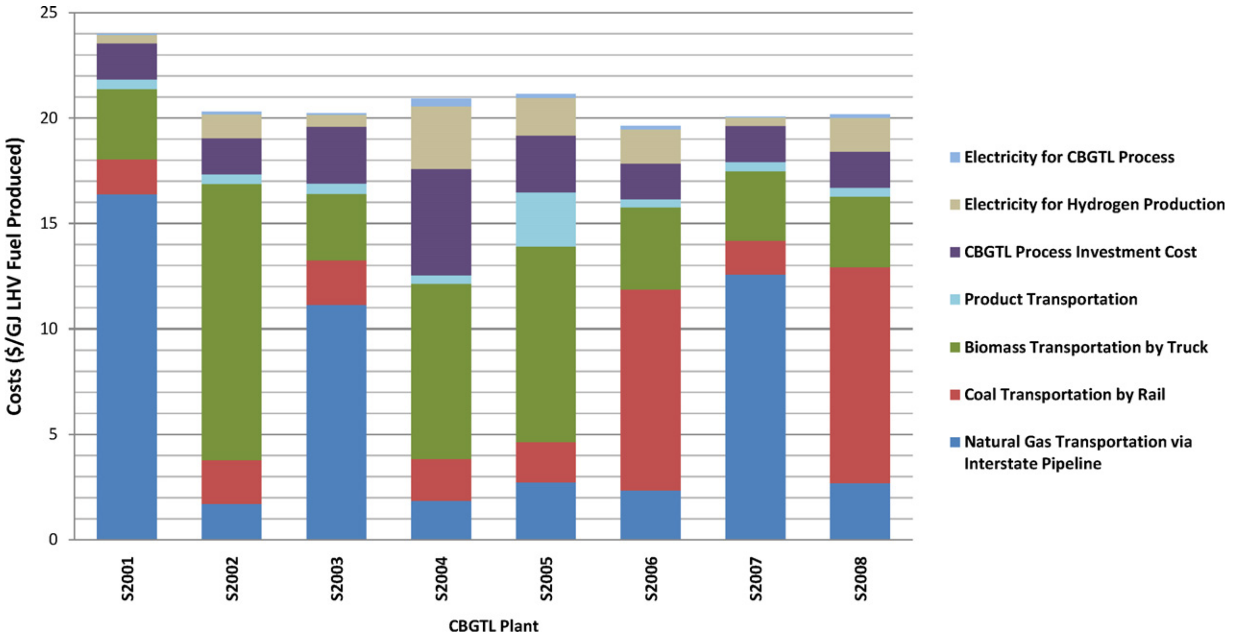

**Fig. 14.** The cost distribution for 8 CBGTL plants in the state of Kansas in the supply chain network for case study 2 with options of carbon-based hydrogen production. All costs for are reported in $/GJ of lower heating value (LHV) of the total products produced. Each facility is represented as S*s* O*o* where *s* represents the FIPS state designation and *o* represents the octant for the particular state. The coal, biomass, natural gas (NG), and hydrogen feedstock prices represent "as-received", delivered to the plant gate prices for the corresponding method of transportation. The levelized investment cost of each facility is based on the fixed capital charges and operating/maintenence costs resulting from the total overnight capital of each plant.

coal feedstock for hydrogen production is constrained to be same as the selected feedstock type of the CBGTL process. For example, if a plant utilizes switchgrass and lignite coal as the biomass and coal feedstocks for the CBGTL process, respectively, the plant must also utilize switchgrass if hydrogen is produced from biomass and lignite coal if hydrogen is produced from coal. The following subsections describe the properties of the updated energy supply chain network in detail.

### 7.2.1. Individual facility costs

The updated optimization model selects 204 CBGTL plants for the network, with 64 small, 103 medium, and 37 large plants. Compared to case study 1, this case study shows over 1,000,000 BPD decrease of fuel production in medium plants, about 800,000 BPD increase of fuel production in large plants, and about 200,000 BPD increase of fuel production in small plants. The marked increase in the number of small plants signifies that a more distributed network is preferred to keep the overall transportation cost for the network at a minimum. The selected CBGTL plants, however, still need to fulfill the same amount of demands for the entire country, which causes the increase in the number of large plants in the supply chain network.

The average cost of the system is $19.94/GJ LHV fuel produced ($100.83/bbl), and the average cost for each plant size is $21.90/GJ ($111.99/bbl) for small plants, $18.84/GJ ($94.56/bbl) for medium plants, and $19.64/GJ ($99.12/bbl) for large plants. While the cost distribution for each CBGTL facility in the previous case study is generally uniform across all facilities, in this study, we see more drastic variations on which segment actually dominates the cost from facility to facility (see Fig. 14). For discussion purposes, Fig. 14 only shows the 8 selected facilities in the state of Kansas, which is selected as a representative state because it contains facilities that utilize biomass, coal, and natural gas as hydrogen feedstock. The dominating cost is either due to the transportation of coal, biomass, or natural gas to the facility, depending on the selected technology for hydrogen production. For example, facilities *S*2002, *S*2004, and *S*2005 have a large segment for biomass delivery due to the selection of biomass as the hydrogen feedstock. Similarly, facilities *S*2001, *S*2003 and *S*2007 have a dominant segment due to natural gas delivery by pipeline and facilities *S*2006 and *S*2008 due to coal delivery. We also note that the investment cost now includes the technology to produce hydrogen and the electricity cost is divided between the cost associated with the CBGTL process and the hydrogen production process.

The plants with the lowest costs of fuel production are located in IL (3 large), IN (1 large), OH (1 medium, 3 large), and VA (1 medium). All of these plants utilize coal reforming technology for hydrogen production and their costs range from $12.28 to $13.87/GJ LHV fuel produced ($57.12–$66.23/bbl). The plants with the highest costs of production are located in AL (2 large), AR (1 large), FL (1 medium), ID (1 medium), LA (1 medium), MS (1 large), and WA (2 medium), with their costs ranging from $27.36 to $36.71/GJ LHV fuel produced ($143.11–$196.40/bbl). The cheaper facilities are located in closer proximity to the coal mines, making it profitable to select coal technology as the hydrogen production option. Since coal is also the cheapest feedstock, the combined effect is that these facilities can produce transportation fuels with lower overall costs. The more expensive facilities, on the other hand, tend to (i) utilize biomass technology and steam reforming of methane to produce hydrogen, or (ii) utilize coal technology and are located far away from coal mines.

We take the most expensive facility in the network as a point of discussion to illustrate the resulting changes in the supply chain network when feedstock availabilities for hydrogen production are taken into account. Facility *S*1204 in FL, a medium-sized plant that utilizes biomass reforming, has the highest cost of $36.71/GJ LHV fuel produced ($196.40/bbl) in the network. In case study 1, three medium-sized plants are selected in the northern part of FL. In case study 2, however, only one medium-sized plant is selected, and this plant is located in the southern part of the state. Because resource availabilities for hydrogen production and their delivery to the plants are taken into account, potential plants in FL must then select one of three technologies whose inputs are the cheapest for them. Coal and natural gas are not available in FL and their loca-

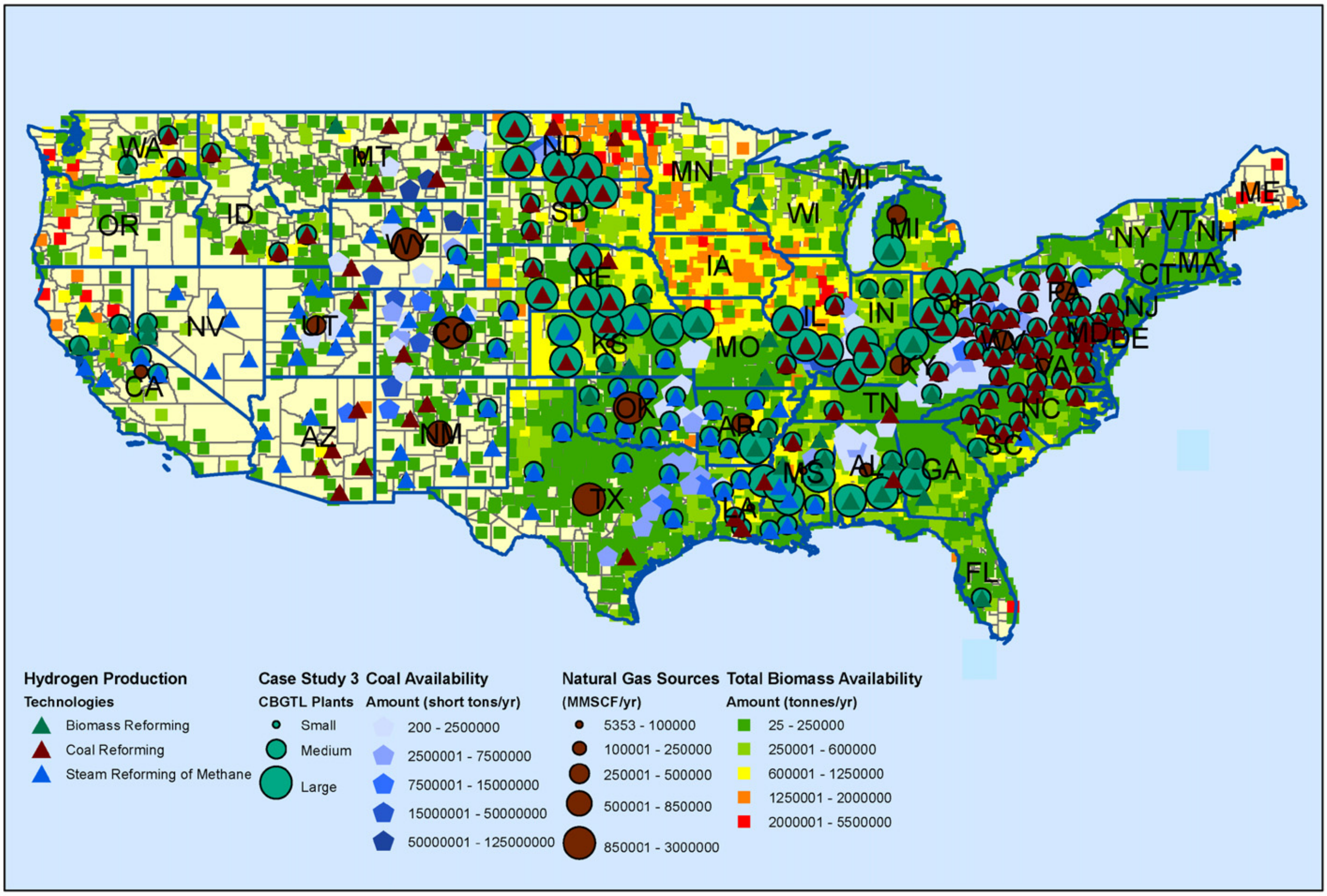

**Fig. 15.** Case study 2 selected facility locations with on-site hydrogen production from biomass, coal, or natural gas. Each facility is represented by a green circle centered at the proposed facility location, with the size of the circle signifying the size of the plant, and a triangle whose color depends on the selected hydrogen producing technology for that specific facility. Due to the overlapping of symbols, some circles may not be displayed on the map, so readers should note that a facility exists wherever a triangle appears. The amounts of coal, biomass, and natural gas feedstock in the United States are also represented as the background of the map. The brown circles signify the sources of natural gas, the blue pentagons represent coal sources, and the green, yellow, and red squares signify biomass sources. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

tions are quite distant from the state (the facility receives coal by rail from WV and natural gas by pipeline from TX). Biomass (generic crop residue), however, is available in FL and is more abundant in the southern part of the state, which is where the selected plant is located. The plant uses biomass reforming to produce hydrogen, and the large amount of biomass that needs to be transported to the plant contributes primarily to the high cost of fuel production for this plant.

### 7.2.2. *Network layout*

With the increased amount of required feedstock to the CBGTL facility sites, now the network layout is even more affected by the locations of coal, biomass, and natural gas sources. The marked difference between the network layout of the previous case study and case study 2 includes, (i) growing fuel production in ND, SD, and OH with the increase of large plants in the region, (ii) significant reduction of fuel production in MO, (iii) more centralized production in AL with the change from medium plants to fewer large plants, and (iv) additional medium plants in WA (see Fig. 15). The locations of the large plants in case study 2 also differ from previous case study, consisting of 5 large plants in KS, 4 in NE, ND, and OH, 3 in IL, KY, MS, and AL, and 2 in SD.

The plants in ND and SD utilize coal reforming of hydrogen production, while the MO plants utilize both coal and biomass reforming. The shifts in production in these states may be due to relatively more abundant resources around ND and SD facilities. ND is abundant in coal and biomass and is able to partially fulfill its own coal requirements and mostly fulfill ND and SD biomass demands. The majority of coal for ND and SD comes from MT and natural gas comes entirely from WY. MO feedstock requirements, on the other hand, have to be fulfilled by more diverse source locations, with some coming from as far as CO and MN. OH is also abundant in coal, as well as possessing biomass and natural gas resources within the state, which gives it more advantage in this case study. The plants in AL, which utilize mostly biomass reforming for hydrogen production, requires many other states to supply its biomass requirement. Even though large amount of biomass delivery will increase the overall cost of the plants, the model determines that it is more profitable to shift AL production to larger plants than to maintain the same amount of production in the neighboring states. Compared to the results from case study 1, we observe a reduction in the number of plants in MS, TN, GA, and FL. Thus, the increased production in AL is necessary to meet the fuel demands in the area.

Except for WA and WI, the states that do not have selected facilities in their regions follow the pattern seen in case study 1. However, the regions from which these states receive liquid fuel products differ from the previous studies due to the changes in the network topology itself. For example, while previously IA receives gasoline, diesel, and kerosene from MO, KY, CO, and KS, in this case study IA receives fuels from ND and SD. The large facil-

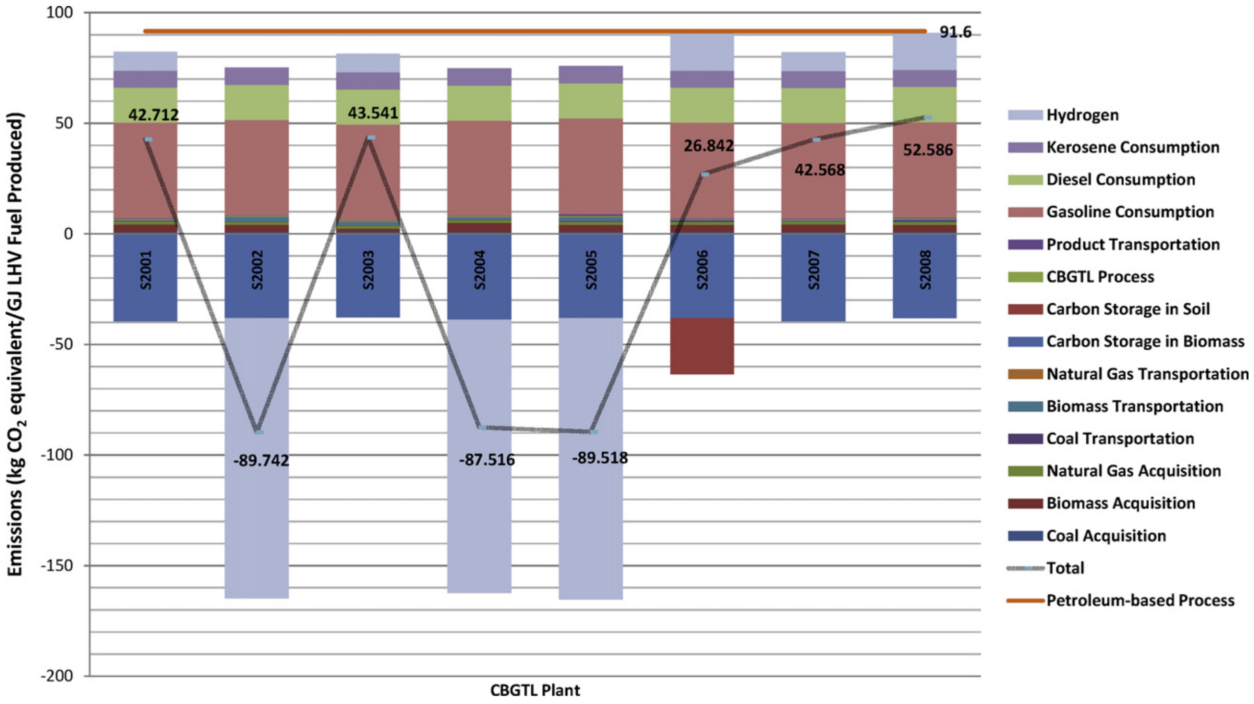

**Fig. 16.** The life cycle analysis of 8 selected facilities in the state of Kansas for case study 2 with three alternatives of hydrogen production technologies, namely hydrogen production from coal, biomass, and natural gas. The current emissions for petroleum based processes is equal to 91.6 kg $CO_{2eq}$/GJ fuel and is represented by the orange bar. The total emissions for each facility is represented by the blue square along the connecting black line and the variation depends on the hydrogen technology selected for each facility. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

ities in MO that previously supply gasoline for IA are reduced in the current network. The facilities in WA are selected in this case study to deliver products to its neighboring locations. They draw their coal sources from MT, natural gas from WY, and biomass locally and from neighboring states. The one facility in WI draws its coal sources from OH, natural gas from WY, and biomass locally, and from MN and ND. These facilities, however, are among the expensive ones in the network with an average cost of $27.31/GJ ($142.83/bbl) for WA and $26.01/GJ ($135.42/bbl) for WI, which explains why they were not selected in the previous case study. The overall movements of feedstock and products across regions are presented in Table 11.

### 7.2.3. Hydrogen production technology selection

Out of the three options of hydrogen production technologies, the network selects 102 plants that utilize coal, 36 for biomass, and 66 for natural gas. Among the plant sizes, 10, 21, and 33 small plants utilize biomass, coal, and natural gas, respectively. The numbers for medium and large plants are 17, 57, 29, and 9, 24, 4 for biomass, coal, and natural gas, respectively. The average costs of facilities are $22.29/GJ ($114.22/bbl) for biomass, $21.63/GJ ($110.46/bbl) for natural gas, and $18.03/GJ ($89.04/bbl) for coal technologies. It makes intuitive sense that coal is the predominant feedstock for hydrogen since it is the cheapest feedstock out of the three, with natural gas second, and biomass last. Natural gas delivered cost is higher than that of coal due to the high price of the commodity itself, and biomass delivered price is high due primarily to its transportation cost. For this reason, it is expected that the medium and large plants lean toward coal as the hydrogen feedstock since they require larger delivered amounts. The distribution of technologies among the medium-sized plants follow the overall pattern with coal being the most used and biomass the least. For large plants, the network selects more biomass technologies than natural gas, which reflect the trade-offs between biomass and natural gas delivered prices depending on the facility locations. For small plants, the numbers of each technology are more evenly distributed, with natural gas plants being the highest in number. The small plants also tend to be located in areas with large distances to the source of one or two feedstock types.

Fig. 15 outlines the layout of how the hydrogen producing technology varies across the country. Naturally, the facilities that utilize coal and natural gas are placed in locations close to the coal mines and natural gas wells, respectively, and the facilities that utilize biomass are mostly clustered in CA, MS, AL, and GA (along with a few in IN, AR, WA, MT, WI, FL, and OK), where coal and natural gas are not as abundant.

### 7.2.4. Life cycle analysis

We assumed that hydrogen production is coupled with $CO_2$ sequestration, and the overall $CO_2$ emissions are 1.53 kg $CO_2$/kg hydrogen for steam reforming of methane, 3.00 kg $CO_2$/kg hydrogen for coal technology, and −22.91 kg $CO_2$/kg hydrogen for biomass technology (National Research Council, 2004). All figures are taken from the current scenarios of each technology according to the NRC report.

Depending on the selection of hydrogen producing technology, the total GHG emissions from each facility vary widely. The life cycle analysis for 8 selected facilities in the state of Kansas is depicted in Fig. 16. Facilities *S*2002, *S*2004, and *S*2005 utilize biomass as the hydrogen feedstock and gain significant emissions reduction from the carbon storage in the biomass feedstock. Facilities *S*2001, *S*2003, and *S*2007 utilize natural gas as the hydrogen feedstock, and the emissions profile look similar to that in case study 1. Facility *S*2008 utilize coal as hydrogen feedstock, yielding the highest emissions figure for Kansas. Facility *S*2006 also utilize coal but is able to obtain lower emissions due to the additional carbon storage in soil from the switchgrass utilization.

Generally speaking, the highest emitting plants utilize coal as hydrogen feedstock, with the highest value being 57.57 kg $CO_{2eq}$/GJ LHV fuel produced, emitted from facility *S*5408, a medium-sized plant in WV. Other high emitting plants are located in DE, MD, MO, NC, OH, PA, and VA. The most notable difference in this case study is the use of biomass as hydrogen feedstock, which provides a large number of negative emissions. Facilities that employ biomass-based technology for hydrogen production have net negative emissions with an average of $-91.31\,\mathrm{kg\,CO_{2eq}/GJ}$ LHV, while the average for coal is $50.23\,\mathrm{kg\,CO_{2eq}/GJ}$ LHV and for natural gas, $41.73\,\mathrm{kg\,CO_{2eq}/GJ}$ LHV. The lowest emitting plants utilize switchgrass as biomass feedstock both for the CBGTL process and hydrogen production, and are located in AL, AR, GA, and MS.

Due to the distinctions between the hydrogen producing technologies, the trade-off between cost and environmental performance in this case study is more marked. The facilities that utilize biomass and natural gas are superior in terms of their environmental impact, but they are also associated with high cost in the whole supply chain network. On the contrary, coal facilities have lowest overall costs, but their average emissions are above the target of 50% petroleum based processes emissions.

## 8. Conclusion

We consider an energy supply chain network to fulfill the United States transportation fuel demands using the hybrid CBGTL process. A mixed-integer linear optimization problem was developed to determine the optimal energy supply network that gives the minimum overall cost of producing transportation fuels, selecting one combination out of the fifteen representative biomass compounds, six coal compounds, one natural gas composition, and three production capacities considered for each CBGTL facility. CBGTL plant parameters are obtained by completing Aspen Plus simulations for each of the feedstock and plant size combination, and the locations and availabilities of feedstocks and transportation infrastructures are obtained from government based databases. The supply chain is assumed to begin at the feedstock locations, ending at the centroid of each state as the final destination of product allocation.

Results of the optimization model reveal that it is more profitable to produce transportation fuels in medium and large plants, since these plants gain more economies of scale. A high number of large plants are located in the midwestern region of the United States, where biomass is abundant. Overall, transportation fuels can be supplied at a cost between \$15.68 and \$22.06/GJ LHV fuel produced (\$76.55–\$112.91/bbl) using carbon-based hydrogen production, with hydrogen production and biomass transportation being the most costly factors in the cost distribution for each facility. The variation in the overall cost for each facility depends on its geographical location and its proximity to the feedstock and product destination locations. The environmental performance of the CBGTL supply chain network is assessed via a life cycle analysis for each facility. The CBGTL process, coupled with carbon-based hydrogen production with sequestration, proves able to fulfill demands with significantly lower GHG emissions than petroleum based processes, meeting the 2050 target of 50% reduction in emissions. In the cases where biomass is used as feedstock for hydrogen production, net negative emissions can be achieved for the facility. As hydrogen and biomass production cost decreases, the CBGTL supply chain network will be both more profitable and environmentally beneficial in the future.

## Acknowledgement

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## Appendix A. Life cycle analysis sample calculation

To evaluate the environmental impacts of new transportation fuels, Argonne National Laboratory (ANL) has developed a spreadsheet-based model that estimates greenhouse gas (GHG) emissions from various fuel production pathways and vehicle/fuel systems (Argonne National Laboratory, 2007). This model is known as the Greenhouse gases, Regulated Emissions, and Energy use in Transportation (GREET) and it calculates (i) the total energy use in various pathways from consuming non-renewable (petroleum, natural gas, and coal) and renewable sources, (ii) the emissions of three main GHGs ($CO_2$, $CH_4$, and $N_2O$), and (iii) the emissions of six pollutants (i.e., volatile organic compounds (VOCs), carbon monoxide (CO), nitrogen oxide (NOx), particulate matter with smaller size than 10 μm (PM10), particulate matter with smaller size than 2.5 μm (PM2.5), and sulfur oxides (SOx)) (Argonne National Laboratory, 2007).

The energy and emissions impact of the CBGTL supply chain network are evaluated by conducting a well-to-wheel life cycle analysis for each plant utilizing parameters given in the GREET model. This cycle includes the processes upstream and downstream of the CBGTL facilities. More specifically, it includes (a) biomass, coal, and natural gas acquisitions, (b) transportation of feedstock from their source locations to the plant facility, (c) carbon storage in the biomass feedstock, (d) carbon storage in the soil and root during biomass cultivation, (e) hydrogen and electricity production, (f) the CBGTL process, (g) transportation and distribution of products, and (h) consumption of fuel products. In this appendix, the parameters used in the calculations, assumptions used, and a sample calculation of the life cycle analysis are outlined.

First, the emissions of the three GHGs (i.e., $CO_2$, $CH_4$, and $N_2O$) are combined in a $CO_2$ equivalent emission figure using their respective global warming potentials (GWPs). The GWP values in the version of the GREET model used in this paper and as recommended by the Intergovernmental Panel on Climate Change Fourth Assessment Report (IPCC AR4) for the 100-year time horizon are as follows: 1 for $CO_2$, 25 for $CH_4$, and 298 for $N_2O$ (Intergovernmental Panel on Climate Change, 2007). In other words, one unit of $CH_4$ emissions, for example, is equivalent to 25 units of $CO_2$ emissions.

VOC, CO, and NOx are among the compounds that have indirect GWPs. According to the IPCC report, the uncertainties associated with indirect GWPs are much greater than direct GWPs (Intergovernmental Panel on Climate Change, 2007). These compounds tend to have short lifetimes in the atmosphere and have nonlinear chemistry in ozone chemistry. Additionally, the indirect effect of NOx can be a negative number and it varies widely with emitting regions, increasing the uncertainty in GWP values. Due to the uncertain values of indirect GWPs for VOC, CO, and NOx, and the possible negative effects of NOx, we exclude these components from the emissions calculation in this study, as does the GREET model.

The next set of parameter values used in the calculations of GHG emissions is the specifications from the various processes that are associated to the CBGTL facilities. Table A.1 presents the emissions from the acquisition of biomass, coal, and natural gas. These numbers are multiplied by their respective GWPs to calculate the total emissions due to each process. For example, the emissions due to natural gas recovery and processing is calculated as follows:

$$\begin{aligned}\text{Natural gas recovery emissions} &= 1(241.8445\,\mathrm{g\,CO_2/kg})\\ &\quad +25(5.5449\,\mathrm{g\,CO_2/kg}) + 298(0.0038\,\mathrm{g\,CO_2/kg})\\ &= 381.5899\,\mathrm{g\,CO_2/kg}\text{ natural gas}\end{aligned} \tag{A.1}$$

The sample calculation in this section is based on large facility *S*105 (located in AL) selected in case study 1 with fixed hydrogen price of \$1.00/kg that takes medium-volatile bituminous coal,

**Table A.1**
Emissions from various processes and modes of transportation associated with the operation of the CBGTL plant. Greenhouse gas emission figures are obtained from the GREET model.

| | VOC | CO | NOx | $CH_4$ | $N_2O$ | $CO_2$ | Total $CO_{2eq}$ | Total carbon |
|---|---|---|---|---|---|---|---|---|
| *Process* | | | | | | | | |
| NG recovery and processing (g/kg) | 0.2652 | 0.3442 | 0.9906 | 5.5449 | 0.0038 | 241.8445 | 381.5899 | 70.6343 |
| Coal mining and cleaning (g/kg) | 0.1594 | 0.0192 | 0.0472 | 2.6881 | 0.0003 | 19.9398 | 87.2344 | 7.6060 |
| Biomass – herbaceous farming and collection (g/dry kg) | 0.0888 | 0.1520 | 0.3714 | 0.0638 | 0.2636 | 57.6542 | 137.8001 | 15.9765 |
| Biomass – forest residue collection (g/dry kg) | 0.0498 | 0.2414 | 0.4720 | 0.0777 | 0.0009 | 67.0202 | 69.2176 | 18.5840 |
| Biomass – agricultural residue collection (g/dry kg) | 0.0430 | 0.1237 | 0.2791 | 0 | 0 | 139.22 | 139.22 | 37.97 |
| *Mode of transportation* | | | | | | | | |
| Barge (g/tonne-mile) | 0.037 | 0.101 | 0.853 | 0.085 | 0.002 | 75.31 | 77.971 | 20.721 |
| Rail (g/tonne-mile) | 0.033 | 0.092 | 0.636 | 0.044 | 0.001 | 35.51 | 36.877 | 9.824 |
| Truck (g/tonne-mile) | 0.047 | 0.217 | 0.466 | 0.127 | 0.003 | 105.73 | 109.673 | 29.157 |
| Pipeline (g/tonne-mile) | 0.012 | 0.059 | 0.251 | 0.049 | 0.001 | 24.70 | 26.104 | 6.834 |

switchgrass, and natural gas. The feedstock and product flowrates associated with this facility are listed in Table A.2. All emissions figures will be normalized to the total lower heating values of the products, whose values are 5.505, 6.145, and 5.982 GJ/bbl for gasoline, diesel, and kerosene, respectively. A large plant produces a total of 200,000 barrels per day (BPD) of products, consisting of 133,534.88 BPD gasoline, 43,201.57 BPD diesel, and 23,263.55 BPD kerosene products. These amounts translate to 8.51 GJ/s of gasoline, 3.07 GJ/s of diesel, and 1.61 GJ/s of kerosene, giving a total of 13.19 GJ/s fuel produced by the facility.

Based on the input flowrates, the emissions due to the acquisition of feedstocks can be calculated as follows, using parameters given in Table A.1:

$$\begin{aligned} &\text{Coal acquisition} \\ &= \frac{(\text{coal input flow rate})(\text{emissions due to coal acquisition})}{\text{total LHV of fuel products}} \\ &= \frac{93.03\,\text{kg/s}\cdot(87.2344E-3)\,\text{kg}\,CO_{2\,\text{eq}}/\text{kg}}{13.19\,\text{GJ/s}} \\ &= 0.615\,\text{kg}\,CO_{2\,\text{eq}}/\text{GJ} \end{aligned} \tag{A.2}$$

**Table A.2**
Input and output streams of facility *S*105 from case study 1 with fixed hydrogen price of $1.00/kg.

| Feedstock/product | Flow rate (kg/s) |
|---|---|
| Medium-volatile bituminous coal | 93.03 |
| Switchgrass | 310.23 |
| Natural gas | 49.35 |
| Hydrogen | 73.34 |
| Gasoline | 184.73 |
| Diesel | 67.17 |
| Kerosene | 33.02 |

$$\begin{aligned} &\text{Biomass acquisition} \\ &= \frac{(\text{biomass input flow rate})\,(\text{emissions due to biomass acquisition})}{\text{total LHV of fuel products}} \\ &= \frac{310.23\,\text{kg/s}\cdot(137.8001E-3)\,\text{kg}\,CO_{2\,\text{eq}}/\text{kg}}{13.19\,\text{GJ/s}} \\ &= 3.241\,\text{kg}\,CO_{2\,\text{eq}}/\text{GJ} \end{aligned} \tag{A.3}$$

$$\begin{aligned} &\text{Natural gas acquisition} \\ &= \frac{(\text{natural gas input flow rate})\,(\text{emissions due to natural gas acquisition})}{\text{total LHV of fuel products}} \\ &= \frac{49.35\,\text{kg/s}\cdot(381.5899E-3)\,\text{kg}\,CO_{2\,\text{eq}}/\text{kg}}{13.19\,\text{GJ/s}} \\ &= 1.427\,\text{kg}\,CO_{2\,\text{eq}}/\text{GJ} \end{aligned} \tag{A.4}$$

Emissions due to the transportation of feedstock to the CBGTL facility and the delivery of products to the demand locations are calculated using the parameters given in Tables A.1 and A.3. Table A.1 specifies the emissions due to a certain mode of transportation and Table A.3 gives the average amounts of how much each mode of transportation is used to deliver a certain commodity and the average distances traveled by each mode of transportation. For example, to deliver coal to power plants, 90% of the time it is transported by rail and the rest is transported by barge. When barges are used, the average distance traveled is 330 miles, while the value is 440 miles for railway and 50 miles for truck. We can then calculate the average distance traveled to transport a commodity for a specified application by multiplying the usage percentages with their respective distances. For example, the average distance for coal transportation is as follows:

$$\text{Distance} = 90\%\cdot 440\,\text{miles} + 10\%\cdot 330\,\text{miles} = 429\,\text{miles} \tag{A.5}$$

**Table A.3**
Delivery assumptions for intermodal transportation as obtained from the GREET model.

| Feedstock | Internodal transport percentage | | | | Internodal transport miles | | | |
|---|---|---|---|---|---|---|---|---|
| | Barge | Rail | Truck | Pipeline | Barge | Rail | Truck | Pipeline |
| Coal – power plant | 10% | 90% | 0% | 0% | 330 | 440 | 50 | 0 |
| Biomass – perennial grasses | 0% | 50% | 50% | 0% | 0 | 440 | 40 | 0 |
| Biomass – forest residues | 0% | 50% | 50% | 0% | 0 | 440 | 75 | 0 |
| Biomass – agricultural residues | 0% | 50% | 50% | 0% | 0 | 440 | 30 | 0 |
| NG – power plant | 0% | 0% | 0% | 100% | 0 | 0 | 0 | 375 |
| Diesel transportation – interstate | 6% | 7% | 0% | 87% | 520 | 800 | 0 | 400 |
| Kerosene transportation – interstate | 6% | 7% | 0% | 87% | 520 | 800 | 0 | 400 |
| Gasoline transportation – interstate | 33% | 7% | 0% | 60% | 520 | 800 | 0 | 400 |
| Diesel distribution – intrastate | 0% | 0% | 100% | 0% | 0 | 0 | 30 | 0 |
| Kerosene distribution – intrastate | 0% | 0% | 100% | 0% | 0 | 0 | 30 | 0 |
| Gasoline distribution – intrastate | 0% | 0% | 100% | 0% | 0 | 0 | 30 | 0 |
| $CO_2$ transport | 0% | 0% | 0% | 100% | 0 | 0 | 0 | 65 |

The emissions due to the transportation of coal would be the product the emission specifications for the modes of transportation, multiplied by the distance traveled and the amount of coal being transported. The calculation steps are similar for biomass, natural gas, and the fuel products:

$$\begin{aligned}
&\text{Coal transportation}\\
&= \frac{(\text{coal input flow rate})\,(\text{average emissions of coal transportation})}{\text{total LHV of fuel products}}\\
&= (93.03E-3)\,\text{tonne/s}\cdot(90\%\cdot 440\,\text{miles}\\
&\cdot(36.877E-3)\text{kg}\,\text{CO}_{2\,\text{eq}}/\text{tonne-miles} + 10\%\cdot 330\,\text{miles}\\
&\cdot(77.971E-3)\,\text{kg}\,\text{CO}_{2\,\text{eq}}/\text{tonne-miles})/13.19\,\text{GJ/s}\\
&= \frac{(93.03E-3)\,\text{tonne/s}\cdot 17.176\,\text{kg}\,\text{CO}_{2\,\text{eq}}/\text{tonne}}{13.19\,\text{GJ/s}}\\
&= 0.121\,\text{kg}\,\text{CO}_{2\,\text{eq}}/\text{GJ} \qquad (\text{A.6})
\end{aligned}$$

We assumed that hydrogen and electricity are produced from coal at a ratio of 1.664 MW feed/MW LHV products, and $CO_2$ is vented from hydrogen and electricity production at a ratio of 12.744 g $CO_2$/MJ LHV products. These values are the average of five different systems from Chiesa et al. (2005) Fuel products were assumed to be transported via interstate pipelines and distributed via intrastate pipelines to the final demand locations.

We note that the distances given in Table A.3 represent the average values for each mode of transportation as given by the GREET model and the above calculations were used to determine the appropriate feedstock compositions for each facility before the Aspen Plus simulations were conducted. In other words, the average distances traveled for each feedstock and product were assumed using the values in Table A.3 because the actual location source and the distance were not known. This, however, is not the case in the solution of the mathematical model. In the optimization model, we assumed that the transportation of feedstock and products are not limited by the values given in the GREET model. Hence in the final life cycle analysis, the distance between origin and destination of each commodity can be calculated explicitly. Facility *S*105, for example, receives coal from locations within the same state by railway. The following equation shows the emissions from one of the locations that deliver coal to facility *S*105:

$$\begin{aligned}
&\text{Coal delivery}\\
&= \frac{(\text{rail emissions})\,(\text{distance traveled})\,(\text{coal input flow rate})}{\text{total LHV of fuel products}}\\
&= \frac{(36.877E-3)\,\text{kg}\,\text{CO}_{2\,\text{eq}}/\text{tonne-mile}\cdot 193.2122\,\text{miles}\cdot(7.568E-3)\,\text{tonne/s}}{13.19\,\text{GJ/s}}\\
&= 0.0041\,\text{kg}\,\text{CO}_{2\,\text{eq}}/\text{GJ} \qquad (\text{A.7})
\end{aligned}$$

**Table A.4**

Coal feedstock sources to facility *S*105 from case study 1 with fixed hydrogen price of $1.00/kg.

| Location | Flowrate (kg/s) | Distance (mi) | Emissions ($kg\ CO_{2eq}/s$) |
|---|---|---|---|
| 1 | 7.5679 | 193.2122 | 0.0539 |
| 2 | 16.2658 | 247.9663 | 0.1487 |
| 3 | 9.7533 | 151.2051 | 0.0544 |
| 4 | 45.2499 | 125.1762 | 0.2089 |
| 5 | 14.1930 | 166.2112 | 0.0870 |

Table A.4 shows the origins of coal feedstock to facility *S*105 and their corresponding emissions values. The total emissions due to coal transportation for facility *S*105 is 0.0419 kg $CO_{2eq}$/GJ. Note that this figure is smaller than the previous calculation with the assumed average distance because the model selects the coal locations that are close to the facility.

The calculations for the transportation of biomass, natural gas, and fuel products also follow the same steps. We also note that gasoline, diesel, and kerosene can be transported via barges. Once the products are delivered to the ports from the various CBGTL facilities, they are mixed and distributed to the demand locations. The amount of emissions attributed to each contributing facility is proportional to the amount of products that the facility sends to the ports.

Biomass utilization in the production of transportation fuels provides negative emissions in the overall fuel life cycle because of the carbon accumulation via photosynthesis that takes $CO_2$ from the atmosphere. The total amount of $CO_2$ taken from the atmosphere during biomass cultivation can be calculated by taking the carbon content of each biomass type (see Table 2), multiplied by the ratio of the molecular weight of $CO_2$ and elemental carbon. The carbon content of switchgrass on a dry basis is 46.9%, so the amount of $CO_2$ taken from the atmosphere during cultivation is the following:

$$\begin{aligned}
\text{CO}_2\text{taken} &= \frac{(\text{biomass input flow rate})(1-\text{moisture content})(\text{carbon content})(\text{MW}\,\text{CO}_2/\text{MW}\,\text{C})}{\text{total LHV of fuel products}}\\
&= \frac{310.23\,\text{kg/s}\cdot(1-0.082)\cdot(0.469)\cdot(44.01/12.01)}{13.19\,\text{GJ/s}} = 37.10\,\text{kg}\,\text{CO}_2/\text{GJ} \qquad (\text{A.8})
\end{aligned}$$

Negative emissions due to biomass soil storage can only be claimed for herbaceous energy crop (i.e., 31.3% kg carbon/kg dry biomass) because its cultivation adds to the current agricultural portfolio (Tilman et al., 2006). Other agricultural and forestal products are currently already in use as food commodities, thus the $CO_2$ uptake due to the land use is already accounted for in the current measurements of $CO_2$ level in the atmosphere. Therefore, the soil sequestration for all other biomass types is taken to be equal to zero. Soil sequestration for switchgrass is calculated by simply multiplying the amount of dry switchgrass (i.e., without moisture content) by 31.3% and the molecular weight ratio of $CO_2$ and elemental carbon:

$$\begin{aligned}
&\text{Soil sequestration}\\
&= \frac{(\text{biomass input flow rate})(1-\text{moisture content})(\text{soil storage})(\text{MW}\,\text{CO}_2/\text{MW}\,\text{C})}{\text{total LHV of fuel products}}\\
&= \frac{310.23\,\text{kg/s}\cdot(1-0.082)\cdot(0.313)\cdot(44.01/12.01)}{13.19\,\text{GJ/s}}\\
&= 24.76\,\text{kg}\,\text{CO}_2/\text{GJ} \qquad (\text{A.9})
\end{aligned}$$

The CBGTL process vents 0.5% of its total carbon input due to the limitation of the Rectisol unit that separates $CO_2$ from the flue gas stream from the fuel combustor unit (Baliban et al., 2010). Using the carbon contents given in the ultimate analysis of each feedstock, the CBGTL emissions for facility *S*105 is 0.336 kg $CO_{2eq}$/GJ. The fuel products are assumed to be combusted fully upon consumption and all of its carbon content will end up in the atmosphere. The normalized values of product emissions are uniform for all facilities and are calculated to be 43.235, 15.819, and 7.758 kg $CO_{2eq}$/GJ for gasoline, diesel, and kerosene consumption, respectively. The consumption of the fuels accounts for the most significant GHG emissions amount in the whole fuel life cycle.

Finally, emissions due to hydrogen and electricity production are calculated based on the production technology used. For renewable production of hydrogen and electricity, GHG emissions are

**Table A.5**
Total $CO_2$ emissions for facility S105 from case study 1 with fixed hydrogen price of $1.00/kg.

| Segments | Emissions (kg $CO_{2eq}$/GJ) |
|---|---|
| Coal acquisition | 0.615 |
| Biomass acquisition | 3.241 |
| Natural gas acquisition | 1.427 |
| Coal transportation | 0.042 |
| Biomass transportation | 0.308 |
| Natural gas transportation | 0.064 |
| Biomass feedstock storage | −37.102 |
| Biomass soil sequestration | −24.761 |
| CBGTL process | 0.336 |
| Product transportation (direct) | 0.115 |
| Product transportation (facility to port) | 0.038 |
| Product transportation (port to port) | 0.066 |
| Product transportation (port to demand location) | 0.008 |
| Gasoline consumption | 43.235 |
| Diesel consumption | 15.819 |
| Kerosene consumption | 7.758 |
| Hydrogen production | 8.311 |
| Total | 19.520 |

taken to be equal to zero. In case study 1, hydrogen is assumed to be produced via steam reforming of methane, which emits 1.53 kg $CO_2$/kg hydrogen with sequestration and 9.22 kg $CO_2$/kg hydrogen without sequestration. Assuming that the hydrogen producers sequester $CO_2$, the emissions due to hydrogen is given by the following equation:

$$\begin{aligned}&\text{Hydrogen emission}\\&=\frac{\text{(emissions of hydrogen production technology)(hydrogen input flow rate)}}{\text{total LHV of fuel products}}\\&=\frac{1.53\,\text{kg}\,CO_2/\text{kg}\cdot 73.34\,\text{kg/s}}{13.19\,\text{GJ/s}}\\&=8.311\,\text{kg}\,CO_{2\,\text{eq}}/\text{GJ}\end{aligned} \tag{A.10}$$

Additional technologies are considered in case study 3 and their emission values are 18.76 kg $CO_2$/kg hydrogen for coal technology without sequestration, 3.00 kg $CO_2$/kg hydrogen for coal technology with sequestration, 2.06 kg $CO_2$/kg hydrogen for biomass technology without sequestration, and −22.91 kg $CO_2$/kg hydrogen for biomass technology with sequestration (National Research Council, 2004).

Table A.5 records all the contributing factors to the total $CO_2$ emissions for facility S105, which is calculated to be 19.520 kg $CO_{2eq}$/GJ, much lower than the emission of petroleum-based processes (91.6 kg $CO_{2eq}$/GJ).

## Appendix B. Abbreviations

### B.1. General abbreviations

| Abbreviation | Description |
|---|---|
| CBGTL | Coal, biomass, and natural gas to liquids |
| GHG | Greenhouse gas |
| FT | Fischer–Tropsch |
| rWGS | Reverse water-gas-shift |
| GREET | Greenhouse gases, regulated emissions, and energy use in transportation |
| ECN | Energy Research Centre of the Netherlands |
| EIA | Energy Information Administration |
| NASS | National Agricultural Statistics Service |
| DOA | Department of Agriculture |
| CRP | Conservation Reserve Program |
| FFS | Federal Forest Service |
| LV | Low-volatile |
| MV | Medium-volatile |
| HV | High-volatile |
| LHV | Lower heating value |
| BEA | Business economic area |
| FIPS | Federal Information Processing Standard |
| TOC | Total overnight cost |
| BOP | Balance of plant |
| IC | Indirect cost |
| DFC | Distance fixed cost |
| DVC | Distance variable cost |
| RM | Refiner's margin |
| BEOP | Break-even oil price |

### B.2. Mathematical model abbreviations

| Abbreviation | Description | Abbreviation | Description |
|---|---|---|---|
| *Indices* | | | |
| $s$ | State index | $c$ | County index |
| $f$ | Feedstock index | $p$ | Product index |
| $t$ | Plant size index | $l$ | Plant location index |
| $m$ | Transportation mode index | $r$ | Port index |
| $h$ | Hydrogen technology index | | |
| *Sets* | | | |
| $S$ | U.S. States | $C$ | U.S. Counties |
| $F^{B-fr}$ | Forest biomass feedstocks | $F^{B-cr}$ | Agricultural biomass feedstocks |
| $F^B$ | Biomass feedstocks | $F^C$ | Coal feedstocks |
| $F^G$ | Natural gas feedstocks | $F$ | feedstocks |
| $FC$ | Feedstock triplets | $P$ | Products |
| $C_F$ | Feedstock-county pairs | $C_P$ | Product-county pairs |
| $M$ | Modes of transportation | $M_F$ | Feedstock-mode pairs |
| $M_P$ | Product mode pairs | $M^G_{Pipe}$ | Natural gas pipelines |
| $M^P_{Pipe}$ | Product pipelines | $R$ | Ports |
| $T$ | Plant sizes | $L$ | Plant locations |
| $EFL$ | Enumerated facility locations | $FL$ | Filtered facility locations |
| $FT$ | Feasible feedstock flow quadruplets | $PT$ | Feasible product flow quadruplets |
| $H$ | Hydrogen production methods | $FL_H$ | Filtered facility locations (with $H_2$ production) |

| Abbreviation | Description |
|---|---|
| *Parameters* | |
| $Prod_t$ | Amount of total fuel products for CBGTL plant size $t$ |
| $Ratio_p$ | Relative proportion of product $p$ from CBGTL plant |
| $N$ | Maximum number of CBGTL plants built in the United States |
| $N_t^{\max}$ | Maximum number of CBGTL plants for size $t$ |
| $N_t^{\min}$ | Minimum number of CBGTL plants for size $t$ |
| $FR^C_{f,f',f'',t}$ | CBGTL coal requirement for feed combination $(f, f', f'')$ and size $t$ |
| $FR^B_{f,f',f'',t}$ | CBGTL biomass requirement for feed combination $(f, f', f'')$ and size $t$ |
| $FR^G_{f,f',f'',t}$ | CBGTL natural gas requirement for feed combination $(f, f', f'')$ and size $t$ |
| $HR_{f,f',f'',t}$ | CBGTL $H_2$ requirement for feed combination $(f, f', f'')$ and size $t$ |
| $ER_{f,f',f'',t}$ | CBGTL electricity requirement for feed combination $(f, f', f'')$ and size $t$ |
| $FA_{f,c}$ | Availability of feedstock $f$ in county $c$ |
| $DM_{p,c}$ | Demand of product $p$ in county $c$ |
| $MaxCost^{FE}_f$ | Maximum delivered cost of feedstock $f$ |
| $MaxCost^{PE}_p$ | Maximum delivered cost of product $p$ |
| $Cap_m$ | Flow capacity of natural gas interstate pipeline $m$ |
| $Usage_m$ | Average daily flow currently in use for the natural gas interstate pipeline $m$ |
| $Cost_{H_2}$ | Fixed cost per unit energy of hydrogen |

| Abbreviation | Description |
|---|---|
| $Cost_{El}$ | Fixed cost per unit energy of electricity |
| $Cost^{F}_{f,c}$ | Cost per unit mass of feedstock $f$ at county $c$ |
| $Cost^{FT}_{f,c,l,m}$ | Cost per unit mass flow to transport feedstock $f$ from county $c$ to facility $l$ using mode $m$ |
| $Cost^{PT}_{p,l,c,m}$ | Cost per unit mass flow to transport product $p$ from facility $l$ to county $c$ using mode $m$ |
| $LC_{f,f',f'',t}$ | CBGTL levelized investment cost for feed combination $(f,f',f'')$ and size $t$ |
| $HC_{f,f',f'',t}$ | CBGTL plant $H_2$ cost for feed combination $(f,f',f'')$ and size $t$ |
| $EC_{f,f',f'',t}$ | CBGTL plant electricity cost for feed combination $(f,f',f'')$ and size $t$ |
| $FR^{C-H_2El}_{f,f',f'',t}$ | Coal feedstock requirement for $H_2$/Elec. production at each CBGTL plant |
| $FR^{B-H_2El}_{f,f',f'',t}$ | Biomass feedstock requirement for $H_2$/Elec. production at each CBGTL plant |
| $FR^{G-H_2El}_{f,f',f'',t}$ | Natural gas feedstock requirement for $H_2$/Elec. production at each CBGTL plant |
| $HC_{f,f',f'',t,h}$ | CBGTL plant $H_2$ cost for feed combination $(f,f',f'')$, size $t$, and $H_2$ technology $h$ |
| $EC_{f,f',f'',t,h}$ | CBGTL plant electricity cost for feed combination $(f,f',f'')$, size $t$, and $H_2$ technology $h$ |
| *Variables* | |
| $Cost^{I}_{l}$ | Levelized investment cost of facility $l$ |
| $Cost^{H}_{l}$ | Hydrogen cost of facility $l$ |
| $Cost^{E}_{l}$ | Electricity cost of facility $l$ |
| $x_{f,c,l,m}$ | Flow of feedstock $f$ from county $c$ to facility $l$ using transportation mode $m$ |
| $z_{p,l,c,m}$ | Flow of product $p$ from facility $l$ to county $c$ using transportation mode $m$ |
| $FR_{f,l}$ | Amount of feedstock $f$ required at facility $l$ |
| $y_{f,f',f'',t,l}$ | CBGTL plant binary at location $l$ with feed combination $(f,f',f'')$ and size $t$ |
| $y_{f,f',f'',t,l,h}$ | CBGTL plant binary at location $l$ with feed combination $(f,f',f'')$, size $t$, and $H_2$ technology $h$ |

## Appendix C. Supplementary data

The complete information on the feedstock requirements and the Aspen Plus simulation results for the 270 distinct CBGTL plant types, including all combinations of biomass, coal, and natural gas types and plant sizes, is available as Supporting Information. This includes (1) input requirements for biomass, coal, and natural gas feedstock, (2) hydrogen input requirements, (3) electricity input requirements for each plant type, and (4) the labeling convention for all CBGTL plants in the supply chain network. Additionally, mathematical model results that include the cost distribution and life cycle analysis for each selected facility from all runs is also provided.

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.compchemeng.2011.01.019.

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